

A geometric approach to quantum circuit lower bounds

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What is the minimal size quantum circuit required to exactly implement a specified n -qubit unitary operation, U , without the use of ancilla qubits? We show that a lower bound on the minimal size is provided by the length of the minimal geodesic between U and the identity, I , where length is defined by a suitable Finsler metric on the manifold $SU(2^n)$. The geodesic curves on these manifolds have the striking property that once an initial position and velocity are set, the remainder of the geodesic is completely determined by a second order differential equation known as the geodesic equation. This is in contrast with the usual case in circuit design, either classical or quantum, where being given part of an optimal circuit does not obviously assist in the design of the rest of the circuit. Geodesic analysis thus offers a potentially powerful approach to the problem of proving quantum circuit lower bounds. In this paper we construct several Finsler metrics whose minimal length geodesics provide lower bounds on quantum circuit size. For each Finsler metric we give a procedure to compute the corresponding geodesic equation. We also construct a large class of solutions to the geodesic equation, which we call *Pauli geodesics*, since they arise from isometries generated by the Pauli group. For any unitary U diagonal in the computational basis, we show that: (a) provided the minimal length geodesic is unique, it must be a Pauli geodesic; (b) finding the length of the minimal Pauli geodesic passing from I to U is equivalent to solving an exponential size instance of the closest vector in a lattice problem (CVP); and (c) all but a doubly exponentially small fraction of such unitaries have minimal Pauli geodesics of exponential length.

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I. INTRODUCTION

A. Overview

A central problem of quantum computation is to determine the most efficient way of implementing a desired unitary operation. Although insight into this problem has been obtained for certain specific unitary operations, no useful general techniques for determining the most efficient implementation are known.

The interest in this problem arises from the desire to find classes of unitary operations which can be implemented *efficiently*, i.e., using polynomial resources. Using a non-constructive measure-theoretic argument, Knill [1] has shown that a generic unitary operation requires exponentially many quantum gates even to approximate. Despite this result, no explicit construction of a natural family of unitary operations requiring exponential size quantum circuits is known.

An analogous situation holds classically, where Shannon [2] (see Theorem 4.3 on page 82 of [3]) used a non-constructive counting argument to show that most Boolean functions $f : \{0, 1\}^n \rightarrow \{0, 1\}$ require circuits of exponential size to compute. Despite this result, no explicit construction of a natural family of functions requiring exponential size circuits is known.

The lack of explicit constructions of hard-to-compute operations is symptomatic of the general difficulty en-

countered in proving lower bounds on the computational resources required to synthesize specified classes of operations, both quantum and classical. The most celebrated instance of this difficulty is, of course, the problem of proving $\mathbf{P} \neq \mathbf{NP}$. More generally, computer scientists suspect many separations between computational complexity classes, but techniques to prove them are elusive.

The problem motivating the present paper is inspired by the problems just described, but is more restricted in scope. Suppose U is a special unitary operation on n qubits, i.e., a $2^n \times 2^n$ unitary operation with unit determinant¹. Let \mathcal{G} be a set of unitary gates which is universal on n qubits, e.g., the set of single-qubit unitary operations and any fixed entangling two-qubit gate [4, 5, 6]. We require \mathcal{G} to be *exactly* universal, i.e., the group generated by \mathcal{G} should be $SU(2^n)$, not some dense subset. Then we define $m_{\mathcal{G}}(U)$ to be the minimal number of gates from \mathcal{G} required to exactly synthesize U .

In this paper we explain how to introduce a metric $d(\cdot, \cdot)$ on $SU(2^n)$ such that $d(I, U) \leq m_{\mathcal{G}}(U)$, where I is the n -qubit identity operation. Thus the metric d provides a *lower bound* on the number of gates required to implement U . We define our metric by first specifying a structure known as a *local metric*, which can be thought of as assigning a distance to points nearby on the manifold. This local metric induces a natural notion of curve length, which can then be used to define $d(\cdot, \cdot)$ as the

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¹ In this paper we work mainly with $SU(2^n)$, rather than $U(2^n)$. As a consequence, all unitaries are assumed to have unit determinant, unless otherwise remarked.

infimum over lengths of curves between two points.

B. Motivating ideas

Two key ideas motivate our geometric approach to the problem of proving lower bounds on $mg(U)$. The first idea is that it is easier to minimize a smooth function on a smooth space rather than a general function on a discrete space, and thus whenever possible we replace discrete structures by smooth structures². This is, of course, an idea familiar to any undergraduate: it is far easier to minimize a smooth function defined on the reals than it is to minimize that function when restricted to the integers. The reason, of course, is that the differential calculus enables us to minimize smooth functions on smooth spaces, using the powerful principle that such a function $f(\cdot)$ should be stationary at a minimum, and thus satisfy the equation $f'(x) = 0$.

This observation motivates us to reformulate the problem of finding a minimal quantum circuit — essentially, an optimization over the discrete space of possible quantum circuits³ — with a closely related problem, which we call the *Hamiltonian control problem*. In the Hamiltonian control problem we attempt to minimize a smooth cost function with respect to a smooth set of Hamiltonian control functions. This formulation allows us to apply the principle that a smooth functional is stationary at its minimum. Technically, we carry this out by using the calculus of variations to study the minimal cost Hamiltonian control function. As we describe below, this idea leads naturally to a geodesic equation whose solutions are control functions which are local minima of the cost function.

A second key idea, overlapping the first, motivates our approach. This idea is built on an analogy to the many principles of physics which can be formulated in one of two equivalent ways: a description in which the motion of a particle is described in terms of a local force law, and a description in which motion is described in terms of minimizing some globally defined functional. To make this analogy precise we use the example of test particle motion in general relativity, but similar remarks may be made in many other areas of physics, including classical mechanics (Newtonian versus Lagrangian formulations), and optics (geometric optics versus Fermat's principle).

It is a basic principle of general relativity that test particles move along geodesics of spacetime, i.e., move so as to minimize a globally defined functional, the pseudo-Riemannian distance. This principle turns out to be

equivalent to the particle following the geodesic equation,

$$\frac{d^2x^j}{dt^2} + \Gamma_{kl}^j \frac{dx^k}{dt} \frac{dx^l}{dt} = 0, \quad (1)$$

where x^j are co-ordinates for the position on the manifold, we sum over the repeated indices k and l , and the Christoffel symbols Γ_{kl}^j are real numbers determined by the local geometry of spacetime. This reformulation shows that minimizing the length traversed is equivalent to following what is essentially a local force law: the geodesic equation tells us how a particle ought to accelerate, given its current velocity and the local geometry. More generally, on any Riemannian or pseudo-Riemannian manifold the problem of geodesic motion turns out to be equivalent to following a local force law, the same geodesic equation of Equation (1).

This situation is in sharp contrast to the problem of finding an optimal circuit to compute a function. Suppose someone gives us a partially complete circuit to compute a function, f , and asks us to complete the circuit. In general, there are no useful techniques for determining the best way of completing the circuit, short of an exhaustive search. But given an arbitrarily small arc along a geodesic on a Riemannian manifold, the remainder of the geodesic is completely determined by the geodesic equation. Indeed, provided we know the velocity at some given point the remainder of the geodesic is completely determined by the geodesic equation.

This analogy motivates our formulating the Hamiltonian control problem so that the cost function to be minimized is a local metric structure on a suitable type of manifold, which we shall argue below is a *Finsler* manifold, a type of manifold generalizing the Riemannian manifolds most familiar to physicists. Just as for Riemannian manifolds, we will see that the geodesics on a Finsler manifold are determined by a geodesic equation of the form of Equation (1), but where the coefficients Γ_{kl}^j are a generalized type of Christoffel symbol for the Finsler manifold. Thus, once the initial position and velocity (or any small arc) are known, the remainder of the geodesic is uniquely determined by the geodesic equation.

An important caveat to this otherwise encouraging situation is that while the solutions to the geodesic equation are local minima of the cost function, they may not be global minima⁴. That is, there may be multiple geodesics connecting I and U , and we will see some explicit examples of this later. Nonetheless, the minimal length curve is guaranteed to be a geodesic⁵, and thus geodesic analysis offers a potentially powerful approach to proving lower bounds on $mg(U)$.

² In a related vein, Linial [7] has written a stimulating survey devoted to the use of geometric ideas in combinatorics.

³ Of course, some (though not all) universal gate sets have a smooth structure. By “discrete” we mean here that the application of a quantum gate is a discrete event, and so the number of quantum gates applied is necessarily a non-negative integer.

⁴ The analogous situation in ordinary calculus is, of course, the fact that $f'(x) = 0$ may have multiple solutions.

⁵ For this reason, we use the terms “minimal length curve” and “minimal length geodesic” interchangeably.

C. Structure and main results

The local metric is a right-invariant \mathcal{G} -bounding Finsler metric:

As just described, our strategy is to define and study suitable classes of local metrics on the manifold $SU(2^n)$. What properties should these local metrics have? In order to find a suitable local metric our strategy is to sequentially impose more and more restrictive conditions, motivated by various properties that we desire the minimal length curves to have.

We begin in Section II (Subsections II A and II B), with a simple general argument motivating the use of local metrics as a measure of the cost of implementing a unitary operation. In Section II (Subsection II B) a simple extension of the same argument is used to motivate the condition that the local metric be right-invariant, which corresponds to the physical requirement that the cost of applying a particular Hamiltonian should not depend on when that Hamiltonian is applied, i.e., it is an expression of homogeneity.

In Section II (Subsection II C) we impose the additional requirement that the local metric should be capable of providing lower bounds on gate complexity, i.e., $d_F(I, U) \leq m_{\mathcal{G}}(U)$, where $d_F(I, U)$ is the distance between I and U induced by the local metric, which we denote by F . In particular, we prove a simple theorem, giving sufficient conditions on F in order that the inequality $d_F(I, U) \leq m_{\mathcal{G}}(U)$ hold. We call local metrics satisfying this condition \mathcal{G} -bounding.

Finally, in Section II (Subsection II D) we impose the additional requirement that the local metric have sufficient smoothness and convexity properties to allow the calculus of variations to be applied to study the minimal length curves. We will show that this is equivalent to requiring that the local metric be a Finsler metric.

Finsler metrics are a class of local metrics generalizing the Riemannian metrics familiar to physicists from the study of general relativity. In Riemannian geometry the length of a small displacement on the manifold is determined by the square root of some quadratic form in the displacement. On a Finsler manifold, this special form for the local metric is replaced by a general norm function, subject only to the most general smoothness and convexity properties sufficient to ensure that a second order differential equation holds for the geodesics. Essentially, Finsler metrics may be viewed as the most general class of local metrics giving rise to such a geodesic equation.

Summing up, the main result of Section II (Subsections II A through II D) is that the most suitable local metric structure is a right-invariant \mathcal{G} -bounding Finsler metric.

Construction of local metrics providing lower bounds on $m_{\mathcal{G}}(U)$: In Section II (Subsection II E) we construct three important families of right-invariant \mathcal{G} -bounding local metrics, which we denote F_1, F_p and F_q . As each of these local metrics is \mathcal{G} -bounding, they all give rise to lower bounds on $m_{\mathcal{G}}(U)$, through the results of Subsection II C. However, F_1 and F_p lack some of the

smoothness and convexity properties required by Finsler metrics. In order to analyse F_1 and F_p within the desired framework of Finsler geometry, in Appendix A we construct a parameterized family of right-invariant Finsler metrics $F_{1\Delta}$ and $F_{p\Delta}$, with the property that $F_{1\Delta} \rightarrow F_1$ and $F_{p\Delta} \rightarrow F_p$ as $\Delta \rightarrow 0$. That is, we can approximate F_1 and F_p as well as desired using suitable families of right-invariant Finsler metrics, and thus study them using the geodesic equation of Finsler geometry.

Computing the geodesic equation: In Section III we explain how to compute the geodesic equation for each of our families of right-invariant Finsler metrics $F_{1\Delta}, F_{p\Delta}$, and F_q . The main tool used in the computation of the geodesic equation is a generalization of the Baker-Campbell-Hausdorff formula used by physicists, which is used to accomplish a necessary change of coordinates on $SU(2^n)$. As a simple illustration of the utility of the geodesic equation, in Section III (Subsection III B) we consider the effect ancilla qubits have on the minimal length curves, showing that for Finsler metrics satisfying suitable conditions — F_q is an example of such a Finsler metric — there is a neighbourhood of the identity in which the presence or absence of ancilla qubits does not affect the minimal length curves.

Construction of the Pauli geodesics: In Section IV (Subsections IV A and IV B) we construct a class of curves in $SU(2^n)$ which are geodesics for all three of the Finsler metrics $F_{1\Delta}, F_{p\Delta}$, and F_q . We call these *Pauli geodesics*, as they arise naturally from a class of isometries associated with the Pauli group.

Finding minimal length Pauli geodesics is equivalent to solving an instance of closest vector in a lattice: In general, many geodesics may connect any two points on $SU(2^n)$, and the problem of finding the minimal length curve connecting two points may be viewed as the problem of finding the minimal length geodesic. We show in Section IV (Subsection IV C) that the problem of finding the minimal length *Pauli* geodesic through a unitary U which is diagonal in the computational basis is equivalent to solving an exponential size instance of the closest vector in a lattice problem (CVP), well known from computer science.

This reduction to CVP is perhaps somewhat ironic, given our general philosophy of replacing discrete structures by smooth structures. However, we will see that the CVP instance is far simpler and has a much more elegant structure than the original problem of finding a minimal-size quantum circuit.

The reduction to CVP is only for the problem of finding the minimal length Pauli geodesic, not the minimal geodesic of any type. Also in Subsection IV C, we show that provided there is a *unique* minimal length geodesic through U , then the minimal length geodesic is a Pauli geodesic, and thus the solution of the CVP instance will give the distance $d_F(I, U)$, and so provide a lower bound on $m_{\mathcal{G}}(U)$. Unfortunately, we are not able to say how generically this situation holds. Standard examples of Riemannian manifolds such as the sphere, flat space and

the hyperbolic spaces suggest it may be true of many or perhaps most U . Against this, in Subsection IV E we give an example where the minimal Pauli geodesic is provably *not* the minimal length geodesic of any type.

Minimal length Pauli geodesics of exponential length exist: Using the connection to CVP, in Section IV (in Subsection IV D) we prove that the overwhelming majority of unitaries diagonal in the computational basis have minimal length Pauli geodesics of exponential length. The method of proof is a volume argument, suggested to the author by Oded Regev.

Caveats: Several additional caveats to our results should be made clear.

The first caveat is that although we have made considerable progress understanding the geodesic structure of our local metrics, we are a long way from a complete understanding of either the geodesics or the minimal length curves of those local metrics. As an example of the type of basic question that is still unresolved, we do not even know for sure if minimal curves of exponential length exist.

These difficulties are perhaps not surprising, as in general it is an extremely difficult problem to understand the minimal length geodesics on a manifold. Indeed, there are few manifolds even of Riemannian type for which the geodesics are completely understood. This paper should thus be viewed as a first step toward an understanding of these minimal length geodesics.

The second caveat is that although we show that $d_F(I, U) \leq m_{\mathcal{G}}(U)$ for right-invariant \mathcal{G} -bounding Finsler metrics, F , it is by no means clear how to choose F in such a way as to achieve the desirable property that $m_{\mathcal{G}}(U)$ and $d_F(I, U)$ be polynomially equivalent. I conjecture that all three of $F_{1\Delta}$, $F_{p\Delta}$, and F_q have this property, for suitable parameter choices. The one concrete step in this direction we take is to show that as $\Delta \rightarrow 0$ the distance $d_{F_{1\Delta}}(I, U)$ can be interpreted as the minimal time required to generate U , using a set of control Hamiltonians each of which can be efficiently simulated in the standard quantum circuit model.

The third caveat is a reiteration and extension of the earlier point that while understanding the behaviour of $m_{\mathcal{G}}(U)$ would be extremely interesting in its own right, it is really a toy version of some much more interesting problems in quantum computational complexity. There are three important ways the determination of $m_{\mathcal{G}}(U)$ falls short of the problems of interest in quantum computational complexity: (1) the requirement that the synthesis of U be exact, rather than approximate; (2) the requirement that this synthesis be performed without the benefit of additional workspace, i.e., without ancilla qubits initially prepared in a standard state; and (3) the lack of a uniformity requirement on the circuit implementing U , i.e., there is no requirement that there be a polynomial-time Turing machine efficiently generating a description of the circuit. Obviously it is to be hoped that these shortcomings can be mitigated by future extensions of the present approach.

The fourth caveat is in relation to the presentation of the paper. The paper is intended to be accessible to physicists, mathematicians, and computer scientists, especially those involved in quantum information science, but makes use of ideas from certain areas of mathematics — differential geometry, Finsler geometry, and the vectorization of matrix equations — that may be unfamiliar to many readers. As the goal of the paper is primarily to synthesize a program for investigating quantum lower bounds, rather than to solve specific technical problems previously considered inaccessible, I have included considerable introductory material and references, as well as describing some arguments in considerable detail, in order to make the broad picture as clear as possible.

D. Prior work

We divide prior work up into research from four different points of view: optimal quantum control, universality constructions for quantum circuits, quantum circuit design, and computational complexity theory.

Optimal quantum control. The work most similar in spirit to the present paper comes from the field of quantum control, particularly optimal quantum control. Quantum control is a large field, and we will not attempt to comprehensively survey it here — see, e.g., [8, 9, 10, 11] for an entry into the literature, and further references.

Only a relatively small part of the quantum control literature has been concerned with time-optimal methods for generating unitary operations. These methods may be subdivided into two (overlapping) approaches: those based on geometric control theory, and those based on using the calculus of variations to minimize some global cost functional without a direct geometric interpretation.

The research most closely related to the present paper is the work on geometric quantum control pursued by Khaneja, Brockett and Glaser [12] (see also [13, 14]), by Zhang and Whaley [15], and by Dirr *et al* [16]. We now briefly outline the approach taken in this prior work, in order to contrast it with the approach taken in the present paper.

These prior works formulate the problem of quantum control as the problem of synthesizing a unitary operation U using a time-dependent control Hamiltonian $H = H_d + \sum_j v_j H_j$, where H_j are control Hamiltonians, v_j are real control functions, and H_d is the drift Hamiltonian. The goal is to synthesize U in the minimal possible time. It is assumed that the control functions v_j can be made arbitrarily intense, for no cost, but the Lie group K which they generate is a strict subgroup of the total Lie group $SU(2^n)$. K might be, for example, the space of local unitary operations on n qubits, while H_d is some global entangling Hamiltonian connecting all the qubits [17]. Thus, the time taken to synthesize U is just the total time for which the drift Hamiltonian H_d is applied.

Khaneja *et al* [12] show that this problem is equiva-

lent to finding the minimal length geodesics on the coset space $SU(2^n)/K$, when that space is equipped with a suitable metric structure. Furthermore, they show that in the special case when $SU(2^n)/K$ is a Riemannian symmetric space these geodesics have an exceptionally simply structure that enable the minimal time to be calculated exactly. This is the case, for example, for $SU(4)/SU(2) \otimes SU(2)$.

The power of this approach comes from the connection to the theory of symmetric spaces, which have a beautiful theory that is exceptionally well understood (see, e.g., [18]). This is also its limitation, for it is only in very special cases that $SU(2^n)/K$ is a symmetric space. See, e.g., [13, 14] for a discussion of the limitations on K imposed by this requirement. In practice, Khaneja *et al.*, Zhang and Whaley, and Dirr *et al* were all limited to studying geodesics for special cases where $n \leq 3$. (We note that some closely related results for $n = 2$ have been obtained in [19, 20, 21], using a different approach based on the theory of majorization.)

Our approach is similar in spirit to this prior work, but differs significantly in substance. We do not identify any special subgroup K , and thus work directly with the space $SU(2^n)$, using the general framework of Finsler geometry, rather than the Riemannian geometry of $SU(2^n)/K$. In this framework, we relate the length of the minimal Finsler geodesic to the minimal size quantum circuit. As our interest is motivated by quantum computation, we are primarily interested in the case of an arbitrary number of qubits, n , and we succeed in constructing geodesics valid for any n , and obtaining some general (albeit, limited) results about the minimal length geodesics for arbitrary n .

Optimal control theory has also given rise to a second strand of work related to the present paper, with a rather more extensive literature than the quantum geometric control literature. Rather than reviewing all this literature in detail, we refer the reader to a recent sample [22, 23, 24, 25, 26, 27], and the references therein.

Broadly speaking, the typical setting for this work is the problem of finding the optimal way of generating a one- or two-qubit quantum gate, using a specified Hamiltonian (e.g., a two-level atom coupled to an external electromagnetic field) containing one or more control parameters. An *ad hoc* functional is constructed, representing the cost of generating the gate in terms of quantities such as the power consumed. The calculus of variations is then employed to derive a condition for that functional to be maximized, typically resulting in a two-point boundary value problem for some second order differential equation, which is then solved numerically using iterative techniques. This body of work is thus much more concerned with obtaining numerical results for specific Hamiltonians and specific one- and two-body unitaries, rather than the general n -qubit questions of most interest to us.

Universality constructions for quantum circuits. Researchers working on universality constructions

for quantum circuits have done considerable work optimizing their constructions. This began in the early papers by Barenco *et al* [28] and Knill [1], who showed that the universality constructions in [28] are near-optimal for a *generic* unitary operation. This work has subsequently been improved by many groups; see, for example, [29, 30, 31, 32], and references therein. This line of investigation appears superficially to be closely related to the topic of the present paper, but that appearance is misleading. The reason is that this prior work investigates constructions which are only *generically* optimal, and there is no reason to believe that the constructions obtained in any of these papers will be optimal for any *particular* unitary operation⁶, and thus they cannot be used to deduce lower bounds on the minimal number of circuit elements required to synthesize a specific unitary operation.

Optimal quantum circuit design. Another topic which has attracted considerable prior interest is the design of optimal quantum circuits for specific tasks. This has become a major topic of ongoing investigation; unfortunately no general survey exists, and a list of references would run to many hundreds. However, the key point is that these papers derive optimal or near-optimal circuits only for certain special classes of unitary operations, e.g., Cleve and Watrous' [33] fast parallel circuits for the quantum Fourier transform. Thus this work does not provide a general approach to the problem of finding optimal circuits for unitary operations, nor for the problem of finding lower bounds on the number of quantum gates required to perform a given (but arbitrary) unitary operation.

Computational complexity. The theory of computational complexity exists in large part, of course, to analyse the time cost of computation, in both classical and quantum computing models. General references are [3, 34].

Within quantum computational complexity, the work of most relevance to the present paper is the work on oracle lower bounds, a selection of which may be found in [35, 36, 37]; see also the references therein. The oracle setting offers substantial technical simplifications when compared with the problem of proving unconditional lower bounds on the difficulty of synthesizing unitary operations, but it is also widely regarded as a much less interesting setting. The results in the present paper are much less complete than some of the results obtained in the oracle setting, but have the advantage of being in the unconditional setting.

Within classical computational complexity, it is worth noting a surface resemblance between the present work and the approach to the $\mathbf{P} \neq \mathbf{NP}$ problem due to Mul-

⁶ A notable exception is that the algorithm in [29] does reproduce the fast quantum Fourier transform circuit. However, [29] notes that the construction in that paper is not optimal in general.

muley and Sahoni [38, 39, 40] (see also [41]). This work also uses geometric techniques to address the problem of proving lower bounds. However, the techniques used are from algebraic geometry, based on geometric invariant theory, and thus are not obviously related to the ideas used in the present paper, which are based on Riemann and Finsler geometry.

II. THE HAMILTONIAN CONTROL PROBLEM AND METRICS ON MANIFOLDS

In this section we introduce the *Hamiltonian control problem*, whose goal is to find a time-dependent Hamiltonian $H(t)$ synthesizing U . For a given Hamiltonian we then define a corresponding *cost*, which is a functional of $H(\cdot)$. We argue on general grounds that the cost function ought to arise from a right-invariant Finsler metric on the manifold $SU(2^n)$, and provide general conditions in order that such a cost function provide a lower bound on $m_G(U)$. Furthermore, we introduce several Finsler metrics satisfying these conditions, and discuss how effective each of these Finsler metrics is likely to be as a means of proving quantum circuit lower bounds.

A. The Hamiltonian control problem

Let U be a special unitary operation on n qubits. Our goal is to synthesize U using a traceless⁷ *control Hamiltonian* $H(t)$. It is convenient to expand the control Hamiltonian in terms of the generalized Pauli matrices, which we take to be the set of n -fold tensor products of the single-qubit Pauli matrices, omitting $I^{\otimes n}$. The resulting expansion is:

$$H(t) = \sum_{\sigma} \gamma^{\sigma}(t) \sigma. \quad (2)$$

Note that we always omit the term $\sigma = I^{\otimes n}$ from such sums. The functions $\gamma^{\sigma}(t)$ are known as *control functions*; the $(4^n - 1)$ -dimensional vector $\gamma(t)$ whose entries are the individual control functions $\gamma^{\sigma}(t)$ is known as *the control function*. Sometimes it is convenient to omit the t and just write γ to denote the entire vector-valued control function $\gamma(t)$.

In order that U be correctly synthesized, Schrödinger's equation requires that the control function $\gamma(t)$ satisfies the equations:

$$\frac{dV}{dt} = -iH(t)V; \quad V(0) = I; \quad V(1) = U. \quad (3)$$

⁷ *A priori* there is no need for the Hamiltonian to be traceless. However, by adding a suitable multiple of the identity we can always make the Hamiltonian traceless, and so there is no loss of generality in making this assumption.

We have chosen $t = 0$ as the initial time, and $t = 1$ as the time at which we desire the evolution to reach U . These choices are arbitrary, and it is not difficult to prove that the definition given below of the cost of synthesizing U does not depend on the values chosen for these times.

It is helpful to assume that $\gamma(t)$ is a smooth (i.e., C^{∞}) function of t . We say that a smooth control function γ satisfying Equations (2) and (3) is a *valid* control function generating U .

B. Cost functions and right-invariant local metrics on manifolds

Our goal is to determine the most efficient way of generating U . To make the notion of efficiency precise, we introduce the *cost* $c_f(\gamma)$ associated to a valid control function γ ,

$$c_f(\gamma) \equiv \int_0^1 dt f(\gamma(t)), \quad (4)$$

where $f : \mathbb{R}^{4^n-1} \rightarrow \mathbb{R}$ is a real-valued function of the control function $\gamma(t)$. We study below the properties which f ought to have if $c_f(\gamma)$ is to be a good measure of efficiency.

We now define the *cost* $c_f(U)$ of the unitary U as the infimum of the cost $c_f(\gamma)$ over all valid control functions γ generating U ,

$$c_f(U) \equiv \inf_{\gamma} c_f(\gamma). \quad (5)$$

Note that we will refer to all three of f , $c_f(\gamma)$ and $c_f(U)$ as the cost function, depending on context.

The remainder of this subsection is devoted to arguing that the cost function f is equivalent to a geometric object known as a right-invariant local metric on the manifold $SU(2^n)$.

To make this argument, in II B 1 we begin by noting a few properties that f ought to have, if $c_f(\gamma)$ and $c_f(U)$ are to be good measures of cost. The purpose here is simply to *motivate* the list of properties we will demand of f , and so the discussion focuses on heuristic arguments and intuition building, rather than on rigorous proofs.

Our list of desired properties for f in hand, in II B 2 we move to the framework of differential geometry, and show that with these properties, f corresponds to a right-invariant local metric on $SU(2^n)$. The advantage of moving to this geometric viewpoint is that it allows the well-developed tools and viewpoint of geometry to be applied.

1. Desired properties of the cost function f

Continuity: A background assumption useful in our later arguments is that f be continuous. Obviously this is reasonable on physical grounds.

Positivity: Given the interpretation of $c_f(U)$ as the cost of synthesizing U , we expect that $c_f(U) \geq 0$, with

equality if and only if $U = I$, the identity operation. Using the continuity of f , it is straightforward to see that this is equivalent to the condition $f(y) \geq 0$, with equality if and only if $y = 0$.

Positive homogeneity: Physically, if we double the intensity of the Hamiltonian for a while, but halve the time it is applied, we wouldn't expect the cost to change, as the total effort required is the same. Mathematically, this idea may be expressed by the requirement that f be positively homogeneous, i.e., that $f(\alpha y) = \alpha f(y)$, for any positive real number α , and any vector y .

Achievement of the infimum: Another useful background assumption is that the infimum in the definition of $c_f(U)$ is achieved by some valid control function γ . This is not strictly necessary for the arguments we make below, but it does streamline them.

The triangle inequality: We will argue that f ought to satisfy the triangle inequality, $f(x + y) \leq f(x) + f(y)$. Suppose γ is the control function which minimizes $c_f(U)$. Fix t , and suppose there exist x and y such that $\gamma(t) = x + y$ and $f(x + y) > f(x) + f(y)$. Choose a value $\Delta > 0$ sufficiently small that $f(\gamma(s))$ is effectively constant over the interval $s \in [t, t + \Delta]$. We construct a new modified control function γ_1 which takes the value $2x$ on the interval $[t, t + \Delta/2]$, the value $2y$ on the interval $[t + \Delta/2, t + \Delta]$, and otherwise takes the same values as γ . Note that this function is not valid, since it is neither smooth nor does it exactly satisfy Equations (2) and (3). However, it is easy to regularize γ_1 to produce a control function γ_2 that is valid, and has essentially the same cost. It follows that $c_f(\gamma_2) = c_f(\gamma_1) < c_f(\gamma)$, which contradicts the presumed minimality of γ . This suggests that f should satisfy the triangle inequality $f(x + y) \leq f(x) + f(y)$ for all x and y .

It is worth noting the additional point that if we desire our minimal curves to be unique then the triangle inequality needs to be strict, i.e., $f(x + y) \leq f(x) + f(y)$, with equality if and only if x and y are along the same ray emanating from the origin. If the strict triangle inequality is not satisfied, then γ could be modified to produce a different valid control function γ_2 with the same cost, using an argument similar to that above. This observation will be useful later, in our discussion of Finsler geometry.

Summarizing, we have argued that the cost function ought to satisfy the conditions: $f(y) \geq 0$ with equality iff $y = 0$; f is positively homogeneous, i.e., $f(\alpha y) = \alpha f(y)$ for all positive α ; and the triangle inequality $f(x + y) \leq f(x) + f(y)$. We now show that these conditions imply a correspondence between f and right-invariant local metrics on $SU(2^n)$.

2. Geometric reformulation of the cost function

We assume the reader is familiar with the concepts of elementary differential geometry, and merely review the necessary notation and nomenclature. The reader unfamiliar with any of these concepts is advised to consult

an introductory text such as Isham [42] or Lee [43]. It will also help to have some familiarity with Riemannian geometry — also covered, albeit rather more briefly, in those texts — but this is not as essential.

We denote a smooth (i.e., C^∞) n -dimensional manifold by M ; we typically omit “smooth” and just refer to M as a manifold. We will often denote points on M by x , and local co-ordinate systems by $\phi : S \rightarrow \mathbb{R}^n$, where S is an open subset of M , and ϕ is a homeomorphism of S into a subset of \mathbb{R}^n . The tangent space to M at point x is denoted $T_x M$, and we often use y to denote a vector in a tangent space such as $T_x M$. We write (x, y) to denote an element of the tangent bundle TM . We will have much interest in C^∞ maps $f : M \rightarrow N$ between manifolds M and N , where by C^∞ we mean that all the derivatives of the map f exist and are continuous with respect to any local co-ordinate systems on M and N . We will use the term C^∞ interchangeably with the term “smooth”. A curve on M is a smooth map $s : I \rightarrow M$, where I is an interval in \mathbb{R} . Given such a smooth map $f : M \rightarrow N$, and fixing $x \in M$, we use $f_* : T_x M \rightarrow T_{f(x)} N$ to denote the natural pushforward map connecting the tangent spaces $T_x M$ and $T_{f(x)} N$.

We define a *manifold with local metric* as a manifold M equipped with a function $F : TM \rightarrow [0, \infty)$ such that for each fixed x , the function $F(x, y)$ satisfies: $F(x, y) \geq 0$ with equality iff $y = 0$; $F(x, y)$ is positively homogeneous in y ; and $F(x, y)$ satisfies the triangle inequality in the second variable. F is called the local metric.

So far as I am aware the term “local metric” is not a standard term in geometry, however in this paper we'll find it a useful unifying term that can be specialized to give the standard concepts of a Finsler or Riemannian metric.

We define the *length* of a curve $s : I \rightarrow M$ on a manifold M with local metric F by

$$l_F(s) \equiv \int_I dt F(s(t), [s]_t), \quad (6)$$

where $[s]_t \in T_{s(t)} M$ is the tangent to s at $s(t)$. With this definition the length is invariant under reparameterization of the curve. More precisely, suppose $\phi : I \rightarrow I'$ is a smooth, strictly monotone increasing function taking the interval I onto another interval I' . Then the identity $l_F(s) = l_F(s \circ \phi)$ follows easily from the definition of length, the positive homogeneity of the local metric, i.e., $F(x, \alpha y) = \alpha F(x, y)$, elementary differential geometry, and calculus.

We define the *distance* $d_F(x, x')$ between two points x and x' on M as the infimum of $l_F(s)$ over all curves s connecting x and x' .

To explain the connection between local metrics and the cost function, we need to introduce *locally adapted co-ordinates* on the manifold $SU(2^n)$. We define these co-ordinates as follows. First, fix an *origin* $U \in SU(2^n)$, and define $\psi : \mathbb{R}^{4^n-1} \rightarrow SU(2^n)$ by $\psi(x) \equiv \exp(-ix \cdot \sigma)U$, where σ here is the $(4^n - 1)$ -component vector whose entries are the generalized Pauli matrices. This maps

\mathbb{R}^{4^n-1} onto $SU(2^n)$ in a many-to-one fashion. Supposing S is an open subset of \mathbb{R}^{4^n-1} such that $\psi : S \rightarrow SU(2^n)$ is one-to-one, we define a set of *U-local adapted co-ordinates* to be the inverse function $\phi : \psi(S) \rightarrow S$.

In practice, we shall only be interested in *U-local adapted co-ordinates* for unitary matrices V in some small neighbourhood of U . In such a neighbourhood we may simply define

$$\phi(V)^\sigma \equiv \frac{i \operatorname{tr}(\ln(VU^\dagger)\sigma)}{2^n}, \quad (7)$$

where \ln is the standard branch of the logarithm. We call this co-ordinate system *the U-local adapted co-ordinates*. Note that we will use the terms “*U-local adapted co-ordinates*” and “*local adapted co-ordinates*” interchangeably, with the former preferred when we wish to be specific about the identity of the origin, and the latter preferred when we wish to omit specific identification of the origin.

Any co-ordinate system x^σ for an open neighbourhood of $U \in SU(2^n)$ induces a corresponding *natural co-ordinate system* for the tangent space $T_U SU(2^n)$. This is done by singling out the *natural basis* $(\partial/\partial x^\sigma)_U$ for $T_U SU(2^n)$, and expanding an arbitrary tangent vector $y \in T_U SU(2^n)$ as $y = \sum_\sigma y^\sigma (\partial/\partial x^\sigma)_U$. We refer to the y^σ as the *natural co-ordinates* for y with respect to the co-ordinate system x^σ . We refer to the co-ordinate system (x^σ, y^σ) for $T SU(2^n)$ as a natural co-ordinate system for the tangent bundle $T SU(2^n)$.

Suppose now that V is a unitary for which *U-local adapted co-ordinates* are defined. Then those co-ordinates give rise to a set of natural co-ordinates for $T_V SU(2^n)$, which we call the *natural U-adapted co-ordinates*, or just the *natural adapted co-ordinates*, when it is clear what value U takes. The following proposition gives a way of computing the natural adapted co-ordinates for the vector tangent to a curve.

Proposition 1. *Let $U(t)$ be a smooth curve in $SU(2^n)$. Then (a) $i \frac{dU}{dt} U^\dagger$ is Hermitian, and (b) the natural $U(t)$ -adapted co-ordinates y^σ for the tangent to the curve, $[U]_t \in T_{U(t)} SU(2^n)$, are determined by the equation⁸*

$$y \cdot \sigma = i \frac{dU}{dt} U^\dagger. \quad (8)$$

In particular, we have $y^\sigma = i \operatorname{tr}(\sigma dU/dt U^\dagger)/2^n$.

Proof: There is a sense in which (a) follows from (b), since the y^σ are real, by definition. Nonetheless, it seems worthwhile to include the following brief proof of (a). Using the unitarity of $U(t)$ we have

$$0 = \frac{d(UU^\dagger)}{dt} = \frac{dU}{dt} U^\dagger + U \frac{dU^\dagger}{dt}. \quad (9)$$

Thus $(dU/dt)U^\dagger$ is anti-Hermitian, which proves part (a).

To prove (b), we expand

$$U(t + \Delta) = U(t) + \Delta \left. \frac{dU}{dt} \right|_t + O(\Delta^2) \quad (10)$$

$$= \exp \left(-i \times i \left. \frac{dU}{dt} \right|_t U(t)^\dagger \Delta \right) U(t) + O(\Delta^2). \quad (11)$$

It follows that the natural $U(t)$ -adapted co-ordinates of the tangent $[U]_t$ are determined by Equation (8). \square

Suppose now that we define a local metric F on the manifold $SU(2^n)$ by $F(U, y) \equiv f(\gamma)$, where f is a cost function, and γ is the vector whose co-ordinates are the natural U -adapted co-ordinates of y . With this definition, the conditions for F to be a local metric follow immediately from the conditions we obtained earlier for the cost function f — positivity, positive homogeneity, and the triangle inequality.

Furthermore, observe from Proposition 1 that if $V(t)$ is a solution to Equations (2) and (3), then the natural $V(t)$ -adapted co-ordinates for the tangent to the curve V at the point $V(t)$ are just the control functions $\gamma^\sigma(t)$. It follows that the cost $c_f(\gamma)$ is equal to the length $l_F(V)$ of the curve V on the manifold $SU(2^n)$, and therefore that the cost $c_f(U)$ is equal to the distance $d_F(I, U)$ between the identity operation I and the unitary U .

We can also show that F is an example of a special type of local metric known as a right-invariant local metric. In general, suppose G is any Lie group (such as, for example, $SU(2^n)$), and $F : TG \rightarrow [0, \infty)$ is a local metric defined on G . Then F is *right-invariant* if $F(x, r_{x*}(y)) = F(e, y)$, where e is the Lie group identity, r_x is right multiplication by x , i.e., $r_x(x') = x'x$, and r_{x*} is the pushforward of r_x at e , mapping $T_e G$ to $T_{x*} G$. With this definition, we see that right-invariant local metrics are simply those which are constant in natural adapted co-ordinates, and thus our F is an example of a right-invariant local metric. We note for later use that left-invariant local metrics are defined similarly to right-invariant local metrics, except the invariance is now under left multiplication, and that a local metric which is both left- and right-invariant is said to be *bi-invariant*.

Summarizing, we have argued on general grounds that the cost associated to the synthesis of a unitary operation U ought to be given by the distance $d_F(I, U)$ between the identity I and U , for some right-invariant local metric F .

C. Minimal curves and lower bounds

In this subsection we prove a simple theorem relating geometry to minimal size quantum circuits, giving sufficient conditions for a local metric F to satisfy $d_F(I, U) \leq mg(U)$.

To state the theorem, it helps to first introduce a little more notation and nomenclature. Suppose \mathcal{G} is some set of unitary gates which is exactly universal when acting

⁸ Note the convention, used here and throughout, that the σ in y^σ refers to a specific generalized Pauli matrix, while in $y \cdot \sigma$ it refers to the entire vector of generalized Paulis.

on n qubits. For example, \mathcal{G} might consist of all one- and two-qubit unitary gates which can be written in the form $\exp(-i\alpha\sigma)$, where $0 \leq \alpha \leq 1$ and σ is either a single-qubit Pauli, or a two-qubit Pauli.

Suppose \mathcal{H} is a set of Hermitian matrices such that the map $\mathcal{H} \rightarrow \mathcal{G}$ defined by $H \rightarrow \exp(-iH)$ is one-to-one and onto. As an example corresponding to the set \mathcal{G} defined in the previous paragraph, we have \mathcal{H} consisting of all Hermitian matrices of the form $\alpha\sigma$, where α and σ are as in the definition of \mathcal{G} .

On the tangent bundle $TSU(2^n)$ we write (V, H) to denote the pair consisting of $V \in SU(2^n)$ and the tangent vector $[\exp(-iHt)V]_{t=0} \in T_V SU(2^n)$. This notation should not be confused with the similar notation (V, y) for elements of $TSU(2^n)$ that we've used up to now, and will continue to use when appropriate, where $V \in SU(2^n)$ and $y \in T_V SU(2^n)$. The advantage of the new notation is that it allows us to write $F(V, H)$ to denote the cost of applying the Hamiltonian H at the point $V \in SU(2^n)$.

Finally, suppose F is a local metric on $SU(2^n)$ satisfying $F(V, H) \leq 1$ for all V in $SU(2^n)$, and for all H in \mathcal{H} . Then we say that F is *\mathcal{G} -bounding*. The reason for this nomenclature is provided by the following theorem, which shows that whenever F is \mathcal{G} -bounding, $d_F(I, U)$ provides a lower bound on $m_{\mathcal{G}}(U)$.

Theorem 1. *Suppose \mathcal{G} is an exactly universal gate set on $SU(2^n)$, and \mathcal{H} is a corresponding set of Hermitian matrices, as described above. Suppose F is a \mathcal{G} -bounding local metric on $SU(2^n)$. Then for any fixed U in $SU(2^n)$ the inequality*

$$d_F(I, U) \leq m_{\mathcal{G}}(U) \quad (12)$$

holds.

Proof: Suppose that $U_1 = \exp(-iH_1), \dots, U_{m_{\mathcal{G}}(U)} = \exp(-iH_{m_{\mathcal{G}}(U)})$ is a minimal sequence of quantum gates synthesizing U , where the gates are chosen from \mathcal{G} . We define a curve $V(t)$ between I and U by defining a control function induced by this gate sequence. The definition of the control function is:

$$\frac{\gamma(t) \cdot \sigma}{m_{\mathcal{G}}(U)} \equiv \begin{cases} H_1 & \text{if } 0 \leq t < 1/m_{\mathcal{G}}(U) \\ H_2 & \text{if } 1/m_{\mathcal{G}}(U) \leq t < 2/m_{\mathcal{G}}(U) \\ \dots & \dots \\ H_{m_{\mathcal{G}}(U)} & \text{if } 1 - 1/m_{\mathcal{G}}(U) \leq t \leq 1. \end{cases} \quad (13)$$

This control function gives rise to a curve between I and U by integrating Equations (2) and (3). However, the curve is not smooth, and so the control function is not valid. To correct this we regularize γ to produce a smooth control function γ_1 that also generates U .

We do this regularization using a real-valued smooth function $r(t)$ with the properties that: (a) $r(t) = 0$ for any point t which is an integer multiple of $1/m_{\mathcal{G}}(U)$; (b) $r(t) \geq 0$; and (c) for any integer j the integral of $r(t)$ over the interval $[j/m_{\mathcal{G}}(U), (j+1)/m_{\mathcal{G}}(U)]$ is $1/m_{\mathcal{G}}(U)$. Such a function is easily constructed using the standard techniques of analysis.

We now define a modified control function $\gamma_1(t) \equiv r(t)\gamma(t)$, and the corresponding curve $V(t)$ is defined by integrating Equations (2) and (3). This is now a smooth curve connecting I and U , and the length of the curve is:

$$l_F(V) = \int_0^1 dt F(V(t), \gamma_1(t) \cdot \sigma) \quad (14)$$

$$= \int_0^1 dt r(t) F(V(t), \gamma(t) \cdot \sigma) \quad (15)$$

$$\leq \int_0^1 dt r(t) m_{\mathcal{G}}(U) \quad (16)$$

$$= m_{\mathcal{G}}(U), \quad (17)$$

where we have applied, respectively: the definition of length; the property that a local metric is positively homogeneous in the second variable; the fact that $\gamma(t) \cdot \sigma/m_{\mathcal{G}}(U)$ is in \mathcal{H} , and the assumption $F(V, H) \leq 1$ for all $V \in SU(2^n)$ and $H \in \mathcal{H}$; and, finally, the fact that for any integer j the integral of $r(t)$ over the interval $[j/m_{\mathcal{G}}(U), (j+1)/m_{\mathcal{G}}(U)]$ is $1/m_{\mathcal{G}}(U)$. It follows that $d_F(I, U) \leq m_{\mathcal{G}}(U)$, as claimed. \square

D. Geodesics and Finsler geometry

We have argued that the cost function f corresponds to a right-invariant \mathcal{G} -bounding local metric F on $SU(2^n)$. In this subsection we will argue that if we are to study the function $d_F(I, U)$ using the calculus of variations, then F ought to belong to a special class of local metrics known as Finsler metrics.

To see this, we again start with some heuristic motivating arguments regarding the properties of f , before turning to a discussion of what these properties mean geometrically, i.e., in terms of the local metric F .

Smoothness: In order to apply the calculus of variations, we need to make some smoothness assumptions about the cost function f . Although it is not strictly necessary, we will assume that the cost function is differentiable to all orders away from the origin, i.e., $f(y)$ is a C^∞ function, except at the origin. The reason we exclude the origin from the smoothness requirement is that if f is non-negative and positively homogeneous, as we argued it ought to be earlier, then the only way f can be differentiable at the origin is if it vanishes everywhere.

The strict triangle inequality and the Hessian: We argued earlier that f ought to satisfy the strict triangle inequality. Our assumption that f is also smooth enables us to recast the strict triangle inequality in a more convenient and (almost) equivalent form. We define the $(4^n - 1) \times (4^n - 1)$ *Hessian* matrix whose entries are $H_{\sigma\tau} \equiv \frac{1}{2} \partial^2 f^2 / \partial y^\sigma \partial y^\tau$, where y^σ is our notation for the σ th co-ordinate slot in the function f^2 . It turns out that a necessary condition for the triangle inequality to hold is that the Hessian matrix be a positive matrix. A sufficient condition for the strict triangle inequality to hold is that the Hessian matrix be strictly positive, and this is the condition we shall impose on f .

These conditions are well-understood in the Finsler geometry community, and so we merely outline why these facts are the case, omitting the details. The interested reader is referred to, e.g., Section 1.2 of the book by Bao, Chern and Shen [44] for a more detailed discussion. Our reason for including this brief discussion here is partially motivational, but also because many of the ideas introduced will be needed later, when we discuss the approximation of local metrics by Finsler metrics.

The key concept behind these results is that of the *indicatrix*. The indicatrix of f , denoted S_f , is defined to consist of all those points y such that $f(y) = 1$. The indicatrix generalizes the unit sphere, where f is the Euclidean norm function. We define the *unit ball* B_f for f to consist of all those points y such that $f(y) \leq 1$.

Assuming f is positively homogeneous, it is not difficult to show that the triangle inequality $f(x+y) \leq f(x) + f(y)$ is equivalent to the condition that the unit ball B_f be convex. Under the same condition, the strict triangle inequality is easily seen to be equivalent to the condition that B_f be *strictly* convex, i.e., any line joining two points of B_f should be contained entirely within the interior of B_f , except possibly at the endpoints. Equivalently, the tangent hyperplane to B_f at any point of S_f should only touch a single point of B_f .

How does this geometry relate to the Hessian? Suppose we pick a point y_0 on the indicatrix. Consider the tangent plane, defined to consist of those points y satisfying $\nabla f \cdot y = \nabla f \cdot y_0$. Define $\Delta \equiv y - y_0$. Expanding $f(y) = f(y_0 + \Delta)$ in a Taylor series in Δ and doing some elementary manipulations gives

$$f(y_0 + \Delta) = 1 + \Delta^T H \Delta + O(\Delta^3), \quad (18)$$

where Δ^T indicates the transpose of Δ , and H is the Hessian matrix. Thus, provided the Hessian is strictly positive, it follows that y_0 is the only point in the tangent hyperplane which is also in B_f , and so the the indicatrix is strictly convex, and the strict triangle inequality is satisfied.

The standard terminology is that f is *strongly convex* when the Hessian is strictly positive; this is a stronger condition than strict convexity of f . It is not difficult to find examples where the Hessian is only positive, not positive definite, and yet the strict triangle inequality holds. Essentially, at such points the quadratic terms in $f(y_0 + \Delta)$ may vanish, yet we still have $f(y_0 + \Delta) > 1$, due to the contribution of higher-order terms, ensuring the strict triangle inequality holds. See, e.g., Exercise 1.2.7 of [44].

We will see that there are significant advantages to assuming that the Hessian is strictly positive, i.e., that strong convexity holds. In particular, in Section III we'll see that this is exactly the condition needed to make the geodesic equation a second order differential equation. If the indicatrix is strictly but not strongly convex then the geodesic equation is not a second order differential equation, but one must instead go to higher order equations, which substantially complicates the study of geodesics.

Summarizing, we have argued that the cost function f ought to be smooth away from the origin, and the Hessian of f ought to be strictly positive definite. We now show that this means that the corresponding local metric F on $SU(2^n)$ is a Finsler metric.

Finsler geometry is a well-developed subject, and our treatment here is based on the standard text by Bao, Chern and Shen [44], and on the notes of Álvarez and Durán [45], to which the reader should refer for more details.

To define Finsler metrics it helps to first define the notion of a Minkowski norm, which is a function $N : \mathbb{R}^d \rightarrow [0, \infty)$ which is smooth away from the origin, satisfies $N(y) \geq 0$ with equality if and only if $y = 0$, is positively homogeneous, and strongly convex in the same sense described earlier, i.e., the Hessian matrix $H = (H_{jk})$ whose components are the partial derivatives

$$H_{jk} \equiv \frac{1}{2} \frac{\partial N^2}{\partial y^j \partial y^k} \quad (19)$$

is strictly positive when evaluated at any point $y \in \mathbb{R}^d$.

Informally, a Finsler metric is a family of Minkowski norms on the tangent spaces to the manifold, one norm for each point on the manifold, and such that the Minkowski norms vary smoothly as a function of position on the manifold. More precisely, a *Finsler metric* on a manifold M is a function $F : TM \rightarrow [0, \infty)$ such that $F(x, y)$ is a smooth function of x and y for all x and all $y \neq 0$, and such that for each fixed x , $F(x, \cdot)$ is a Minkowski norm on the tangent space $T_x M$.

Clearly, Finsler metrics are a special case of local metrics. Note also that Riemannian metrics are a special case of Finsler metrics, coinciding with the condition that $F(x, \cdot)^2$ be a quadratic form for each fixed $x \in M$.

When the cost function f is smooth away from the origin and has a strictly positive Hessian, we see that the corresponding local metric⁹ $F(U, y) \equiv f(\gamma)$ is an example of a right-invariant Finsler metric. Thus, the local metrics we shall be most interested in studying in this paper are right-invariant \mathcal{G} -bounding Finsler metrics.

Finsler metrics have a number of useful properties that we note here without proof.

First, the Hopf-Rinow theorem (see page 168 and exercise 6.2.11 on page 155 of [44]) implies that for a compact Finsler manifold the infimum in the definition of d_F is always achieved by some smooth curve.

Second, Euler's theorem for smooth and homogeneous functions (see Section 1.2 of [44]) implies a number of

⁹ Recall that the components of γ are just the natural U -adapted co-ordinates for y .

useful identities satisfied by Finsler metrics:

$$\sum_j \frac{\partial F^2}{\partial y^j} y^j = 2F^2 \quad (20)$$

$$\sum_{jk} \frac{\partial^2 F^2}{\partial y^j \partial y^k} y^j y^k = 2F^2 \quad (21)$$

$$\sum_j \frac{\partial F^2}{\partial y^j \partial y^k \partial y^l} y^j = 0. \quad (22)$$

In these equations, the y^j are any fixed set of co-ordinates for the tangent space $T_x M$. Note that Equation (22) can be recast in several different ways, depending on which order the partial derivatives are taken. We use several of these different orderings later.

E. Examples of local metrics whose minimal length curves provide lower bounds on circuit size

We have argued that if F is to be useful for proving lower bounds on $m_{\mathcal{G}}(U)$ then it ought to be a \mathcal{G} -bounding local metric; even better, a Finsler metric, in order that the calculus of variations and results like the Hopf-Rinow theorem be applicable. In addition to these properties, a local metric F ideally should have the following three properties: (1) it is easy to determine the minimal curve length $d_F(I, U)$; (2) there exist families of unitaries indexed by n and with long minimal geodesics according to F , i.e., families of unitaries for which $d_F(I, U)$ scales exponentially with n ; and (3) $d_F(I, U)$ is polynomially equivalent to $m_{\mathcal{G}}(U)$. Note that (3) implies (2), since unitaries for which $m_{\mathcal{G}}(U)$ is exponential are known to exist [1].

It is a significant open problem to find a local metric satisfying all of these properties.

The purpose of the present subsection is to introduce four natural candidates for such a local metric, denoted F_1, F_2, F_p , and F_q , and to discuss the extent to which they satisfy these desired properties. All of them are right-invariant \mathcal{G} -bounding local metrics, and thus at least satisfy the inequality $d_F(I, U) \leq m_{\mathcal{G}}(U)$.

We will see that one of these local metrics, F_2 , definitely does not have all the desired properties. Although our discussion is not conclusive, it is plausible that each of the other three local metrics does possess the desired properties, with the caveat that F_1 and F_p are not Finsler, and must be approximated by suitable Finsler metrics. In particular, we will present some heuristic evidence that F_1 and F_p satisfy all our criteria.

To define our local metrics let $U \in SU(2^n)$, $y \in T_U SU(2^n)$, and suppose y has natural U -adapted co-ordinates y^σ , and so can be thought of as corresponding

to the Hamiltonian $y \cdot \sigma$. Then we define

$$F_1(U, y) \equiv \sum_{\sigma} |y^\sigma| \quad (23)$$

$$F_2(U, y) \equiv \sqrt{\sum_{\sigma} (y^\sigma)^2} \quad (24)$$

$$F_p(U, y) \equiv \sum_{\sigma} p(\text{wt}(\sigma)) |y^\sigma| \quad (25)$$

$$F_q(U, y) \equiv \sqrt{\sum_{\sigma} q(\text{wt}(\sigma)) (y^\sigma)^2}. \quad (26)$$

In these expressions, $\text{wt}(\sigma)$ is the Hamming weight of the Pauli matrix σ , and $p(\cdot)$ and $q(\cdot)$ are *penalty functions* that penalize the control function whenever Pauli terms of high weight contribute to the control Hamiltonian. E.g., we might choose $p(j) = 4^j$ to provide an exponential penalty for the use of higher-weight Pauli matrices. We return to the choice of the penalty function below.

As was remarked earlier, it is often useful to write $F(U, H) \equiv F(U, y)$, where H is the Hamiltonian such that $y = [\exp(-iHt)U]_{t=0}$. With this convention it is easily verified that right-invariant local metrics such as F_1, F_2, F_p and F_q have no U -dependence, and so we sometimes write $F(H) \equiv F(\cdot, H)$. Note that $F(H)$ is a norm on $su(2^n)$.

We now apply Theorem 1 to these example metrics. To do this, we choose the universal gate set \mathcal{G} as in the example described earlier, specifically, to consist of all one- and two-qubit unitary gates which can be written in the form $\exp(-i\alpha\sigma)$, where $0 \leq \alpha \leq 1$ and σ is a Pauli matrix of weight one or two. The corresponding \mathcal{H} consists of all Hermitian matrices of the form $\alpha\sigma$.

We see immediately that with these choices F_1 and F_2 satisfy the hypothesis of Theorem 1, namely, we have $F_1(V, H) \leq 1$ and $F_2(V, H) \leq 1$ for all $V \in SU(2^n)$ and all $H \in \mathcal{H}$. Thus, we have $d_{F_1}(I, U) \leq m_{\mathcal{G}}(U)$ and $d_{F_2}(I, U) \leq m_{\mathcal{G}}(U)$. In the case of F_p and F_q we need the supplementary assumptions that $p(1), p(2) \leq 1$ and $q(1), q(2) \leq 1$, respectively. With these assumptions it is easily verified that the hypothesis of Theorem 1 holds, and so we have $d_{F_p}(I, U) \leq m_{\mathcal{G}}(U)$ and $d_{F_q}(I, U) \leq m_{\mathcal{G}}(U)$.

1. Properties of F_2 and F_q

F_2 is an example of a very well understood class of local metrics: it is a bi-invariant Riemannian metric on $SU(2^n)$. Such local metrics have the nice property that their geodesics are completely understood — they are the curves of the form $\exp(-iHt)$, where $H \in su(2^n)$ — as are properties such as curvature and other geometric invariants. See, e.g., the end-of-chapter problems in Chapter 5 of [46].

Although F_2 is well understood, it turns out that the lower bounds on $m_{\mathcal{G}}(U)$ obtained from F_2 are at best con-

stant, and thus are not especially interesting. In particular, we will show that for any U we have $d_{F_2}(I, U) \leq \pi^2$, and thus the best possible bound we can hope for is $\pi^2 \leq m_G(U)$.

To see that $d_{F_2}(I, U) \leq \pi^2$, observe first the identity $F_2(V, H) = \text{tr}(H^2)/2^n$. Then for any U , select Hermitian H with eigenvalues in the range $-\pi$ to π and such that $\exp(-iH) = U$. Define a curve γ from I to U via $\gamma(t) \equiv \exp(-iHt)$; this can actually be shown to be the minimal length geodesic through U , although we won't need this fact. The length of this curve is $l_{F_2}(\gamma) = \int_0^1 dt F_2(\exp(-iHt), H) = \text{tr}(H^2)/2^n$. It follows that¹⁰ $d_{F_2}(I, U) \leq \frac{\text{tr}(H^2)}{2^n}$. But from the eigenvalue bounds on H it follows that $\text{tr}(H^2) \leq \pi^2 2^n$, whence we obtain

$$d_{F_2}(I, U) \leq \pi^2. \quad (27)$$

Thus we can never hope to prove any more than that $\pi^2 \leq m_G(U)$ using F_2 .

The essential reason F_2 is unsuitable for proving lower bounds is that it contains no information about the tensor product structure, as can be seen from the expression $F_2(H) = \text{tr}(H^2)/2^n$. How can we encode information about the tensor product structure in the metric, in order to have some hope of obtaining non-constant lower bounds on circuit size? One possibility is to simply exclude the possibility of the control Hamiltonian containing Pauli terms of weight higher than two. To do this we need to move to the field of sub-Riemannian geometry [47], which is concerned with the situation where there are restrictions on the allowed directions that a curve may take in the tangent space. This direction of research is under investigation by the author.

Another possible approach is to introduce a penalty function $q(\cdot)$ which penalizes the use of high weight Pauli matrices in the control Hamiltonian. Many forms for the penalty function suggest themselves, and it is not clear which, if any, is the most appropriate. Here is one illustrative choice:

$$q(j) = \begin{cases} 1 & \text{if } j = 1 \text{ or } 2 \\ k & \text{otherwise,} \end{cases} \quad (28)$$

where k is a penalty that may depend on the number of qubits n , but is otherwise constant. As k becomes large we expect that this approach will yield essentially the same geodesics as in the sub-Riemannian approach mentioned above. One advantage of using such a local metric is that it is a right-invariant Riemannian metric, and such local metrics are quite well understood. See, e.g., Appendix 2 of [48], and the end-of-chapter problems in Chapter 5 of [46].

2. Properties of F_1 and F_p

The local metric F_1 is perhaps the most promising cost function, due to the following interpretation. Suppose U may be generated by applying sequentially the Pauli matrices $\sigma_1, \sigma_2, \dots$ for times t_1, t_2, \dots . Then the length l_{F_1} of the corresponding curve is just the total time $t_1 + t_2 + \dots$. An approximate converse is also true. In particular, using the Trotter formula it is easy to prove that for any Hamiltonian H and time $t \geq 0$ it is possible to approximate $\exp(-iHt)$ arbitrarily well using just Pauli Hamiltonians σ , applied for a total time $F_1(H)t$. It follows that given a curve γ , we can approximate γ arbitrarily well using a sequence of evolutions, each one a Hamiltonian evolution with Hamiltonian some generalized Pauli sigma matrix, with the total time of evolution being just $l_{F_1}(\gamma)$. Note also that Hamiltonian evolution according to any single generalized Pauli matrix is easily simulatable with at most a linear number of gates in the standard quantum circuits model.

Thus, $d_{F_1}(I, U)$ has a natural interpretation as the minimal time required to generate U by switching between Hamiltonians chosen from the set of generalized Pauli matrices, each of which can be efficiently simulated in the standard quantum circuits model.

It is tempting to suppose on the basis of this interpretation that $d_{F_1}(I, U)$ must be polynomially equivalent to $m_G(U)$. Although I believe this likely to be the case, it is possible to imagine, for example, that $d_{F_1}(I, U)$ is small (maybe even a constant), and yet the oscillations in any near-optimal path γ are so wild that to approximate it in the quantum circuit model requires exponentially many gates. If this were the case then the cost in doing the computation would not be due to the actual Hamiltonian evolution, but rather due to extremely frequent switching between very short evolutions by different Pauli Hamiltonians.

In the event that this turns out to be the case, one potential resolution would be to work instead with F_p , in which a penalty function $p(\cdot)$ is used to penalize the use of higher-weight Pauli matrices in the Hamiltonian evolution. As was the case for F_q it is not clear what the best choice of penalty function is, but various simple alternatives naturally suggest themselves. In particular, as for F_q , by choosing p appropriately we can effectively rule out some directions of movement on the manifold. When F_p is by approximated by a suitable Finsler metric (as described in the next paragraph) ruling out such directions of movement places us effectively in the realm of “sub-Finsler” geometry [49, 50].

The main disadvantage of F_1 and F_p is that they are not Finsler metrics, and thus we can't directly apply the calculus of variations to study their minimal length curves. To remedy this situation, in Appendix A we explain how to approximate F_1 and F_p by a family of Finsler metrics $F_{1\Delta}$ and $F_{p\Delta}$, where $\Delta > 0$ is a small parameter such that as $\Delta \rightarrow 0$, $F_{1\Delta} \rightarrow F_1$ and $F_{p\Delta} \rightarrow F_p$. More

¹⁰ As this is the minimal length curve, the inequality which follows is, in fact, an equality.

precisely, we show that

$$F_1(U, y) \leq F_{1\Delta}(U, y) \leq \frac{F_1(U, y)}{1 - (4^n - 1)\Delta}, \quad (29)$$

$$F_p(U, y) \leq F_{p\Delta}(U, y) \leq \frac{F_p(U, y)}{1 - P\Delta}, \quad (30)$$

where $P \equiv \sum_{\sigma} p(\text{wt}(\sigma))$. Thus, provided Δ is sufficiently small the Finsler metrics $F_{1\Delta}$ and $F_{p\Delta}$ provide excellent approximations to F_1 and F_p , respectively. As a result, our strategy for understanding the minimal length curves of F_1 and F_p is to study them via the geodesics of $F_{1\Delta}$ and $F_{p\Delta}$.

3. Summary and comparison

We have introduced four classes of local metric, F_1, F_2, F_p , and F_q . All four provide lower bounds on $m_{\mathcal{G}}(U)$ through the inequality $d_F(I, U) \leq m_{\mathcal{G}}(U)$. Summarizing and comparing their various properties:

1. F_2 is capable of producing at best a constant lower bound on $m_{\mathcal{G}}(U)$, and thus is not especially interesting.
2. F_q is a modified version of F_2 in which we introduce a penalty for the application of higher-weight Pauli Hamiltonians. The main advantages of F_q are that it is easy to compute and Riemannian. It is also straightforward to compute quantities such as curvature and the Christoffel symbols using standard results about right-invariant Riemannian metrics.
3. F_1 is the best motivated of all the four local metrics. In particular, we showed that $d_{F_1}(I, U)$ is the minimal time required to synthesize U using some set of efficiently simulatable Hamiltonians. It can be approximated arbitrarily well using a suitable Finsler metric $F_{1\Delta}$.
4. F_p is a modified version of F_1 in which we introduce a penalty for the application of higher-weight Pauli Hamiltonians. It can also be approximated arbitrarily well using a suitable Finsler metric $F_{p\Delta}$.

I conjecture that for suitable choices of the penalty functions, p and q , all three of the local metrics F_1, F_p , and F_q are polynomially equivalent to $m_{\mathcal{G}}(U)$, and thus could, in principle, be used to prove exponential lower bounds on $m_{\mathcal{G}}(U)$. In this paper we will not resolve the correctness of this conjecture, although Section IV C presents some evidence that F_1 (and thus F_p) has exponential length minimal curves, which provides some indirect evidence for the conjecture.

Despite the lack of a proof of this conjecture, it remains an interesting problem to understand the geodesic structure of each of these classes of local metric, and what this implies about the distances $d_F(I, U)$. It is to this problem that we turn for the remainder of this paper.

III. COMPUTING THE GEODESIC EQUATION

In this section we'll explain how to explicitly construct the geodesic equation for each of the Finsler metrics we have introduced. This equation is a second-order differential equation whose solutions are geodesics of the Finsler manifolds, i.e., curves in $SU(2^n)$ which are local extrema of the Finsler length.

The exact form of the geodesic equation is rather complex, even for the simplest of our local metrics; we shall not write it out explicitly. Our goal in this section is to describe a general procedure which can be used to compute the geodesic equation, and thus enable numerical and analytic investigation of geodesics. A detailed numerical investigation of the geodesic structure is underway and will appear elsewhere.

We begin in Subsection III A, with a brief review of the geodesic equation for Finsler geometry. This is standard material in Finsler geometry, and so we cover it quickly, merely outlining derivations, and referring the reader to standard references such as [44] for more details.

In order to apply the geodesic equation it is most convenient to pick out a single co-ordinate system¹¹ for $SU(2^n)$, and carry out all calculations with respect to those co-ordinates. In particular, using a single set of co-ordinates greatly facilitates integration of the geodesic equation, and analytic investigation of that equation. Unfortunately, the Finsler metrics we have introduced in Subsection II E are all defined in terms of local adapted co-ordinates, which vary from point to point on $SU(2^n)$.

To remedy this situation, the majority of this section is taken up with learning how to change from local adapted co-ordinates to a single fixed set of co-ordinates for $TSU(2^n)$, which we call natural Pauli co-ordinates. We explain how to make this change of variables for the special case of $TSU(2)$ in Subsection III D. In Subsection III E we describe the main ideas behind the change of variables for $TSU(2^n)$, before describing some convenient calculational techniques for making this change in Subsection III F.

With these results in hand it is possible in principle to explicitly compute the geodesic equation for each of the local metrics we have introduced. In practice, the actual form of the equation is rather complicated, and it is more convenient to investigate solutions numerically, or using techniques such as the analysis of symmetries. Indeed, as we do not do any numerical analysis in this paper, later sections of the paper in fact depend only on the basic form of the geodesic equation, presented in Subsection III A, and so the other parts of this section

¹¹ In fact, no single co-ordinate system can cover all of $SU(2^n)$. However, it is possible to pick a co-ordinate system that covers all of $TSU(2^n)$ except a set of measure zero, and that is what we will do. We return later to the question of what to do on the set of measure zero.

may be skipped if the reader's main interest is in the geodesic solutions constructed in Section IV.

The section also contains a brief digression, in Subsection III B, whose purpose is to illustrate the results of Subsection III A with some simple results on the effects ancilla qubits have on minimal length curves. In particular, we show that for a suitable family of Finsler metrics, there is a neighbourhood of the identity in which for all unitaries U the distance $d_F(I, U)$ is equal to the distance $d_F(I \otimes I, U \otimes I)$, i.e., the distance is unaffected by the addition of ancilla on which the unitary acts trivially. These results, simple as they are, represent our only progress on the problem of understanding the effect ancilla qubits have on minimal size quantum circuits.

A. General form of the geodesic equation

In this subsection we construct the geodesic equation. We follow the standard procedure used in Finsler geometry (see, e.g. [44]) to construct the equation, and for that reason we merely outline the relevant calculations.

In order to construct the geodesic equation, it is convenient to fix a set of co-ordinates for $SU(2^n)$. We will label these co-ordinates x^j , and the corresponding natural co-ordinates for the tangent space y^j . The co-ordinate system x^j chosen is a completely arbitrary chart from among the atlas of possible co-ordinates on the manifold. Note that at any point along a curve $s = s(t)$ the tangent vector has natural co-ordinates given by $y^j = dx^j/dt$.

In general, the co-ordinates x^j do not cover all of $SU(2^n)$. As a result, to construct geodesics it is in general necessary to change the co-ordinate system being used as the geodesic moves across the manifold. However, for this initial discussion it is most convenient to imagine that the co-ordinate system has been fixed, and we are computing geodesics that lie within the region covered by that co-ordinate system.

Recall that we defined the length of a curve $s : I \rightarrow M$ by $l_F(s) \equiv \int_I dt F(s(t), [s]_t)$, where $[s]_t \in T_{s(t)}M$ is the vector tangent to s at t . In terms of the co-ordinates x^j and $y^j = dx^j/dt$ this may be rewritten $l_F(s) = \int_I dt F(x, y)$, where $F = F(x, y)$ is F expressed in terms of the co-ordinates $x = (x^j)$ and the corresponding natural co-ordinates $y = (y^j) = (dx^j/dt)$ for the tangent vector $[s]_t$.

In order to determine the geodesics which minimize the length we use the calculus of variations, a review of which may be found in [51]. It is a standard result in the calculus of variations that any curve s which is an extremum of the functional $\int_I dt F(x, y)$ must satisfy the Euler-Lagrange equations:

$$\frac{d}{dt} \left(\frac{\partial F}{\partial y^j} \right) = \frac{\partial F}{\partial x^j}. \quad (31)$$

We will sometimes refer to this equation as the geodesic equation, for its solutions give rise to geodesics. However, for practical purposes it is more convenient to recast

the geodesic equation in other forms. First, and rather remarkably, it is possible to replace F by F^2 in Equation (31) to get an equation which is essentially equivalent:

$$\frac{d}{dt} \left(\frac{\partial F^2}{\partial y^j} \right) = \frac{\partial F^2}{\partial x^j}. \quad (32)$$

To understand this equivalence and its significance, note the easily-verified identity:

$$\begin{aligned} & \left(\frac{d}{dt} \left(\frac{\partial F^2}{\partial y^j} \right) - \frac{\partial F^2}{\partial x^j} \right) \\ &= 2 \frac{dF}{dt} \frac{\partial F}{\partial y^j} + 2F \left(\frac{d}{dt} \left(\frac{\partial F}{\partial y^j} \right) - \frac{\partial F}{\partial x^j} \right). \end{aligned} \quad (33)$$

Suppose $s = s(t)$ is a curve which solves the geodesic equation, Equation (31). Then we can reparameterize this curve to give an equal length curve \tilde{s} which has constant speed, i.e., $dF/dt = 0$ along the curve \tilde{s} . It is straightforward to verify that the curve \tilde{s} also solves the geodesic equation, Equation (31). However, since $dF/dt = 0$, we see from Equation (33) that \tilde{s} is also a solution to Equation (32).

Conversely, suppose the curve $s = s(t)$ is a solution to Equation (32). Then we have:

$$\frac{dF^2}{dt} = \sum_j \left(\frac{\partial F^2}{\partial x^j} \frac{dx^j}{dt} + \frac{\partial F^2}{\partial y^j} \frac{dy^j}{dt} \right) \quad (34)$$

$$= \sum_j \frac{d}{dt} \left(\frac{\partial F^2}{\partial y^j} y^j \right). \quad (35)$$

Using Equation (20) we see that $\sum_j \frac{\partial F^2}{\partial y^j} y^j = 2F^2$, and so the previous equation implies $dF^2/dt = 2 dF^2/dt$, and so any solution to Equation (32) automatically satisfies the constant speed condition $dF^2/dt = 0$.

Summing up, the class of curves which solve Equation (31) is equivalent to the class of curves which solve Equation (32), up to a reparameterization which leaves the length invariant, and thus is of no interest. However, solutions to Equation (32) have the additional useful property that they are automatically curves of constant speed. We therefore refer to either Equation (31) or Equation (32) as the geodesic equation, depending on context.

Equation (32) may be recast in an equivalent form analogous to the standard geodesic equation for Riemannian manifolds, Equation (1). First, using Equations (21) we substitute $F^2 = g_{lm} y^l y^m$, where we define $g_{lm} \equiv \frac{1}{2} \frac{\partial F^2}{\partial y^l \partial y^m}$ to be the Hessian, and we use the summation convention that repeated indices are summed over, unless otherwise stated. The right-hand side of Equation (32) then becomes $g_{lm,x^j} y^l y^m$, where we use the subscript notation " $_{,x^j}$ " to indicate a partial derivative with respect to the x^j co-ordinate.

To analyse the left-hand side of Equation (32), we again substitute $F^2 = g_{lm} y^l y^m$, and apply the usual rules

of calculus together with Equation (22) to obtain

$$\frac{\partial F^2}{\partial y^j} = 2g_{jm}y^m. \quad (36)$$

Taking the total derivative with respect to t , and again using Equation (22), we obtain

$$\frac{d}{dt} \left(\frac{\partial F^2}{\partial y^j} \right) = 2g_{jm,x^n}y^m y^n + 2g_{jm} \frac{dy_m}{dt}. \quad (37)$$

Using these results we see that the geodesic equation, Equation (32), may be recast in the form

$$2g_{jm,x^n}y^m y^n + 2g_{jm} \frac{dy_m}{dt} = g_{lm,x^j}y^l y^m. \quad (38)$$

By assumption, the matrix whose components are the g_{jk} is strictly positive, and so it is possible to define a matrix g^{jk} which is the inverse of g_{jk} . Multiplying Equation (38) by this inverse and doing some rearrangement, we obtain our alternate form of the geodesic equation,

$$\frac{d^2x^j}{dt^2} + \Gamma_{kl}^j \frac{dx^k}{dt} \frac{dx^l}{dt} = 0, \quad (39)$$

where the Christoffel symbols Γ_{kl}^j are defined by

$$\Gamma_{kl}^j \equiv \frac{g^{jm}}{2} (g_{mk,x^l} + g_{ml,x^k} - g_{kl,x^m}). \quad (40)$$

Formally, this definition for the Christoffel symbols appears identical to that used in Riemannian geometry. The difference is that in Riemannian geometry the g_{jk} are functions of x alone, while in Finsler geometry they are typically functions of y as well.

Summing up, we have presented the geodesic equation in three different (but equivalent) forms, Eqs. (31), (32), and (39). The latter is explicitly in the form of a second order differential equation, and so the usual existence and uniqueness theorems for second order ordinary differential equations apply. In particular, given an initial position and velocity (i.e., tangent vector) on the manifold, the remainder of the geodesic is completely specified by Equation (39). Of course, this form of initial data problem is not the problem of most interest to us. We are more concerned with the problem of studying geodesics where two points on the geodesic are specified, but the initial velocity is unknown.

B. Application: Ancilla qubits and direct sum theorems

As an illustration of the results of the previous subsection, consider the problem of determining $m_{\mathcal{G}}(U \otimes V)$, where U is a unitary on an n_A -qubit system, labeled A , and V is a unitary on an n_B -qubit system, labeled B . An interesting question is to ask how $m_{\mathcal{G}}(U \otimes V)$ is related to $m_{\mathcal{G}}(U)$ and $m_{\mathcal{G}}(V)$, where the notation

\mathcal{G} is overloaded in the obvious way. It is clear that $m_{\mathcal{G}}(U \otimes V) \leq m_{\mathcal{G}}(U) + m_{\mathcal{G}}(V)$. Might this inequality sometimes be strict, or must it be satisfied with equality?

Questions like this are the province of *direct sum theorems*, which seem to have first been considered by [52]. Essentially, a direct sum theorem seeks to establish whether a set of two or more computational tasks can be collectively accomplished using fewer resources than the sum of the resources required for the individual tasks.

Of particular interest in the context of the current paper is the case $V = I$, which is related to the problem of determining whether or not ancilla can help in implementing U .

With the tools available we cannot directly study the behaviour of $m_{\mathcal{G}}(U \otimes V)$, but we can study the related question of whether $d_{F_{AB}}(I_A \otimes I_B, U \otimes V) = d_{F_A}(I_A, U) + d_{F_B}(I_B, V)$, where F_A, F_B and F_{AB} are suitable Finsler metrics on the respective spaces. We will not solve this problem in general, but can easily obtain some simple results indicating that, at least near the identity, this equality will always be satisfied for suitable choices of the Finsler metrics.

Suppose F_A, F_B and F_{AB} are Finsler metrics on $SU(2^{n_A}), SU(2^{n_B})$ and $SU(2^{n_A+n_B})$, respectively. We say they form an *additive triple* of Finsler metrics if:

$$F_{AB}^2(U \otimes V, H_A + H_B) = F_A^2(U, H_A) + F_B^2(V, H_B), \quad (41)$$

where $H_A \in su(2^{n_A})$, $H_B \in su(2^{n_B})$, and we abuse notation by omitting tensor factors which act trivially, like $I_A \otimes \cdot$ and $\cdot \otimes I_B$.

Suppose $U(t)$ is a geodesic of F_A , and $V(t)$ is a geodesic of F_B . If F_A, F_B and F_{AB} are an additive triple of Finsler metrics, then it follows from the linearity of the geodesic equation, Equation (32), that $W(t) \equiv U(t) \otimes V(t)$ is a geodesic of F_{AB} .

An example of an additive triple of Finsler metrics is the triple F_{q_A}, F_{q_B} , and $F_{q_{AB}}$, where the penalty functions q_A, q_B and q_{AB} satisfy the consistency condition $q_A(j) = q_B(j) = q_{AB}(j)$, for all j where this condition is well-defined. It follows that if $U(t)$ and $V(t)$ are geodesics of F_{q_A} and F_{q_B} , then $U(t) \otimes V(t)$ is a geodesic of $F_{q_{AB}}$.

We have seen that a tensor product of geodesic curves is itself a geodesic curve, for additive triples of Finsler metrics. Can we conclude that the shortest curve connecting $I_A \otimes I_B$ and $U \otimes V$ is just the tensor product of the shortest curve connecting I_A and U with the shortest curve connecting I_B and V ?

I do not know if this is the case, in general. However, a well-known theorem of Finsler geometry (see, e.g., Section 6.3 of [44]) asserts that for any manifold M equipped with a Finsler metric F , there exists a constant $r > 0$ such that any geodesic of length less than r is guaranteed to be a minimal length curve.

It follows that for U and V in some finite-size neighbourhood of the respective identity operations, I_A and I_B , the minimal curve from $I_A \otimes I_B$ to $U \otimes V$ is just

the tensor product of the minimal curves in the respective spaces. It follows that in this neighbourhood the distance $d_{F_{AB}}(I_A \otimes I_B, U \otimes V)$ is equal to the sum $d_{F_A}(I_A, U) + d_{F_B}(I_B, V)$.

Specializing to the case where $V = I_B$, we see that for all U in some finite-size neighbourhood of I_A the minimal length curve from $I_A \otimes I_B$ to $U \otimes I_B$ is guaranteed to be exactly equal to the minimal length curve from I_A to U . That is, there is a neighbourhood of the identity in which the presence of ancilla does not help in shortening the length of the minimal curves.

C. Pauli co-ordinates

As noted in the introduction to this section, our primary goal in this section is to explain how to compute the geodesic equation with respect to a fixed co-ordinate system on $SU(2^n)$. The co-ordinates we shall use are the Pauli co-ordinates. In our earlier language, Pauli co-ordinates are I -adapted local co-ordinates for $SU(2^n)$, where I is the n -qubit identity operation. The unitary corresponding to Pauli co-ordinates x is given by

$$\exp(-ix \cdot \sigma) = \exp\left(-i \sum_{\sigma} x^{\sigma} \sigma\right). \quad (42)$$

Inverting, the co-ordinates x^{σ} corresponding to some unitary U are given by

$$x^{\sigma} \equiv \frac{i \operatorname{tr}(\ln(U)\sigma)}{2^n}, \quad (43)$$

where \ln is some branch of the logarithm. We will be particularly interested in the case where \ln is the standard branch of the logarithm, defined around a branch cut along the negative real axis. We call these co-ordinates the *standard Pauli co-ordinates*, or just Pauli co-ordinates. Note that the standard Pauli co-ordinates are defined for any unitary operator whose spectrum does not include -1 , and thus are defined everywhere in $SU(2^n)$ except on a set of measure zero.

Just as for local adapted co-ordinates, the Pauli co-ordinates on $SU(2^n)$ give rise to natural co-ordinates on the tangent space $T_U SU(2^n)$. In the remainder of this section we will typically use x^{σ} to denote Pauli co-ordinates, \tilde{x}^{σ} to denote local adapted co-ordinates, and y^{σ} and \tilde{y}^{σ} to denote the corresponding natural co-ordinates on $T_U SU(2^n)$.

D. Changing co-ordinates in $T_U SU(2)$

Let's begin with the example of $T_U SU(2)$, where it is relatively straightforward to change between the natural Pauli and natural locally adapted co-ordinates. The key to making the change is the following theorem. Note that in this subsection (and in the associated Appendix B) we

will find it useful to work both with vectors in \mathbb{R}^3 , and with vectors relating directly to objects in the tangent bundle $T_U SU(2)$. We will refer to the former using the notations \vec{x} , \vec{y} and \tilde{y} , while for the latter we will use x to refer to the vector of Pauli co-ordinates for $U \in SU(2)$, and y to refer to an element of $T_U SU(2)$.

Theorem 2. *Fix $\vec{x} \in \mathbb{R}^3$. Then*

$$\begin{aligned} & \exp(-i(\vec{x} + t\tilde{y}) \cdot \sigma) \\ &= \exp(-it\tilde{y} \cdot \sigma) \exp(-ix \cdot \sigma) + O(t^2), \end{aligned} \quad (44)$$

where \tilde{y} may be expressed as a function of \vec{x} and \tilde{y} :

$$\tilde{y} = \tilde{y}_{\parallel} + \|\vec{x}\| \cot(\|\vec{x}\|) \tilde{y}_{\perp} + \tilde{y} \times \vec{x}. \quad (45)$$

In this expression $\hat{x} \equiv \vec{x}/\|\vec{x}\|$ is the normalized vector in the \vec{x} direction, $\tilde{y}_{\parallel} \equiv \hat{x} \cdot \tilde{y} \hat{x}$ is the component of \tilde{y} in the \hat{x} direction, and $\tilde{y}_{\perp} \equiv \tilde{y} - \tilde{y}_{\parallel}$ is the component of \tilde{y} orthogonal to the \hat{x} direction. We can invert this equation to express \tilde{y} in terms of \vec{x} and \tilde{y} , obtaining:

$$\tilde{y} = \tilde{y}_{\parallel} + \operatorname{sinc}(2\|\vec{x}\|) \tilde{y}_{\perp} + \operatorname{sinc}^2(\|\vec{x}\|) \vec{x} \times \tilde{y}_{\perp}, \quad (46)$$

where \tilde{y}_{\parallel} is now the component of \tilde{y} in the \hat{x} direction, \tilde{y}_{\perp} is the component of \tilde{y} orthogonal to \hat{x} , and $\operatorname{sinc}(z) \equiv \sin(z)/z$ is the standard sinc function.

The proof of this theorem is a straightforward calculation. We describe the details in Appendix B. Alternately, it is a useful and not entirely trivial exercise to deduce the theorem from the more general results about $SU(2^n)$ in the next subsection.

To see how this theorem enables us to change co-ordinates, fix $U \in SU(2)$, and fix $y \in T_U SU(2)$. Suppose x are the Pauli co-ordinates for U . Then we have

$$y = \sum_{\sigma} y^{\sigma} \left(\frac{\partial}{\partial x^{\sigma}} \right)_U \quad (47)$$

for some set of co-ordinates y^{σ} , and where $(\partial/\partial x^{\sigma})_U$ are the natural Pauli co-ordinate basis vectors for $T_U SU(2)$. Setting $\vec{x} \equiv x$ and letting \tilde{y} have components y^{σ} , we see that the vector $y \in T_U SU(2)$ is tangent to the curve $\exp(-i(\vec{x} + t\tilde{y}) \cdot \sigma)$ at $t = 0$. That is:

$$y = [\exp(-i(\vec{x} + t\tilde{y}) \cdot \sigma)]_{t=0}. \quad (48)$$

Applying Theorem 2, we obtain

$$y = [\exp(-it\tilde{y} \cdot \sigma)U + O(t^2)]_{t=0}. \quad (49)$$

Neglecting the terms of order t^2 does not change the tangent at $t = 0$, and so

$$y = [\exp(-it\tilde{y} \cdot \sigma)U]_{t=0}. \quad (50)$$

It follows that \tilde{y}^{σ} are the natural adapted co-ordinates for $T_U SU(2)$. Thus Theorem 2 relates the natural Pauli co-ordinates y^{σ} on $T_U SU(2)$ to the natural U -adapted co-ordinates \tilde{y}^{σ} on $T_U SU(2)$.

E. Changing co-ordinates in $T_U SU(2^n)$

The key result enabling the change between natural Pauli and natural locally adapted co-ordinates is a generalization of Theorem 2 which applies to unitary operators in arbitrary dimensions. This result is due to Baker [53], Campbell [54, 55] and Hausdorff [56], and we refer to it as the *BCH formula*. Note that this result is *not* what is usually referred to as the BCH formula by physicists, but is a generalization. See Section 3.4 of [57] for a recent discussion of the BCH formula and related results.

To state the BCH formula it helps to first define linear superoperators (i.e., linear operations on matrices) ad_X and \mathcal{I} by $\text{ad}_X(Z) \equiv [X, Z]$, and $\mathcal{I}(Z) \equiv Z$. With these definitions we have the following.

Theorem 3 (BCH formula). *Suppose X and Y are $d \times d$ Hermitian operators. Then we have*

$$\exp(-it\tilde{Y}) \exp(-iX) = \exp(-i(X + tY)) + O(t^2), \quad (51)$$

where the $d \times d$ Hermitian operator \tilde{Y} is defined by

$$\tilde{Y} \equiv \mathcal{E}_X(Y), \quad (52)$$

and \mathcal{E}_X is a linear superoperator defined by

$$\mathcal{E}_X = \frac{\exp(-i\text{ad}_X) - \mathcal{I}}{-i\text{ad}_X}. \quad (53)$$

In this theorem, the superoperator \mathcal{E}_X is understood as a formal power series. In particular, the operator ad_X is not invertible, so strictly speaking the expression given for \mathcal{E}_X is not even defined. Nonetheless, treating the expressions as power series, we see that

$$\mathcal{E}_X = \sum_{j=0}^{\infty} \frac{(-i\text{ad}_X)^j}{(j+1)!} \quad (54)$$

is defined and everywhere convergent. We will discuss in the next subsection how to explicitly calculate the action of \mathcal{E}_X in a convenient fashion. For now we take it as given that this can be done, and discuss how Theorem 3 allows us to change variables in $T_U SU(2^n)$.

The discussion, of course, follows similar lines to the discussion in the previous subsection. We fix $y \in T_U SU(2^n)$, and suppose \vec{x} is a vector of Pauli co-ordinates for U , so $U = \exp(-i\vec{x} \cdot \sigma)$. We will find it convenient to use x^σ both to denote Pauli co-ordinates, and also the particular Pauli co-ordinates for U , with the meaning to be determined by context. Then we have

$$y = \sum_{\sigma} y^\sigma \left(\frac{\partial}{\partial x^\sigma} \right)_U \quad (55)$$

$$= [\exp(-i(\vec{x} + t\vec{y}) \cdot \sigma)]_{t=0}, \quad (56)$$

where \vec{y} is the vector whose entries are the natural Pauli co-ordinates y^σ . Using the BCH formula we have

$$y = [\exp(-it\tilde{y} \cdot \sigma)U + O(t^2)]_{t=0} \quad (57)$$

$$= [\exp(-it\tilde{y} \cdot \sigma)U]_{t=0}, \quad (58)$$

where \tilde{y} is determined by \vec{x} and \vec{y} through the equations

$$\tilde{y} \cdot \sigma = \mathcal{E}_{\vec{x} \cdot \sigma}(\vec{y} \cdot \sigma) \quad (59)$$

$$\mathcal{E}_{\vec{x} \cdot \sigma} = \frac{\exp(-i\text{ad}_{\vec{x} \cdot \sigma}) - \mathcal{I}}{-i\text{ad}_{\vec{x} \cdot \sigma}}. \quad (60)$$

Note that the components of \tilde{y} may be extracted from this expression by multiplying both sides by some specific Pauli matrix σ and taking the trace.

Equations (59) and (60) are general equations telling us how to transform from natural Pauli co-ordinates in $T_U SU(2^n)$ to natural adapted co-ordinates in $T_U SU(2^n)$. By applying the inverse operation we can transform from natural adapted co-ordinates into natural Pauli co-ordinates. A straightforward but somewhat lengthy calculation shows that in the case where $n = 1$ these results reduce to the results for $SU(2)$ deduced in the previous section. We omit the details of this calculation.

F. Explicit computation of the change of co-ordinates

In the last subsection we explained how to change from natural Pauli co-ordinates to natural adapted co-ordinates in $T_U SU(2^n)$, through Equations (59) and (60). These formulas are compact, but it is not entirely evident how to perform an explicit calculation of this change of co-ordinates. In this subsection we explain how to perform such calculations, and also how to do the inverse change, from natural adapted co-ordinates to natural Pauli co-ordinates. This enables, in principle, the explicit computation of all terms in the geodesic equation, Equation (39).

One way of performing such calculations is to expand $\mathcal{E}_{\vec{x} \cdot \sigma}$ in a power series in $\text{ad}_{\vec{x} \cdot \sigma}$, as specified by Equation (54). Computations can then be carried out to a good approximation simply by computing the first few terms of the power series. Along similar lines, the inverse to $\mathcal{E}_{\vec{x} \cdot \sigma}$ also has a power series expansion (see the discussion in Section 3.4 of [57]), and so computations of the inverse can be carried out along similar lines.

However, there is a useful alternate approach offering the possibility of exact computation, which we now describe. In particular, we will describe a general method to compute $\mathcal{E}_X(Y)$.

There are two main difficulties facing us in the computation. The first is that it is computationally inconvenient to deal with superoperators like ad_X . To alleviate this difficulty we will *vectorize* our expressions. Vectorization is a procedure that converts operators into vectors, and superoperators into operators, to obtain equivalent expressions involving only vectors and ordinary operators. This step is not strictly necessary, but it is extremely convenient. As the vectorization formalism is not entirely standard in the quantum information literature, an introduction to this formalism is presented in Appendix C, to which the reader not familiar with vectorization should now turn.

The second, and more serious, difficulty, is that ad_X is not invertible. Our solution is to decompose Y into a component lying in the kernel of ad_X , and a component lying in the orthocomplement of the kernel. We then compute the action of \mathcal{E}_X on each of these two spaces separately. This computation is also greatly facilitated by use of the vectorization formalism.

We begin with a useful characterization of the kernel of ad_X , which we denote $\ker(\text{ad}_X)$. Recall that $\ker(\text{ad}_X)$ consists of all those matrices Z such that $\text{ad}_X(Z) = 0$. The following proposition gives a computationally convenient description for $\ker(\text{ad}_X)$.

Proposition 2. *Suppose the Hermitian matrix X has spectral decomposition $\sum_j x_j P_j$, where the x_j are the distinct eigenvalues of X , and the P_j project onto the corresponding eigenspaces. Then the operation*

$$\mathcal{P}(Z) \equiv \sum_j P_j Z P_j \quad (61)$$

projects onto the kernel of ad_X .

Proof: To see that \mathcal{P} is a projector we need to show that it is Hermitian and satisfies $\mathcal{P} \circ \mathcal{P} = \mathcal{P}$. Both of these facts are easily verified.

To complete the proof we need to show that $\mathcal{P}(Z) = Z$ if and only if Z is an element of the kernel of ad_X . To prove the forward implication, suppose $\mathcal{P}(Z) = Z$. Then $Z = \sum_j P_j Z P_j$. Thus $\text{ad}_X(Z) = \sum_j [X, P_j Z P_j] = 0$, as required. To prove the reverse implication, suppose $\text{ad}_X(Z) = 0$. Then $[X, Z] = 0$, and we conclude that it must be possible to write $Z = \sum_j Z_j$, where Z_j acts only within the eigenspace corresponding to the eigenvalue x_j . It follows that $\mathcal{P}(Z_j) = Z_j$, and thus $\mathcal{P}(Z) = Z$, as desired. \square

To compute $\mathcal{E}_X(Z)$ we first consider two special cases: the case when Z is an element of $\ker(\text{ad}_X)$, and the case when Z is in the orthocomplement to $\ker(\text{ad}_X)$.

Case: $Z \in \ker(\text{ad}_X)$. We see from inspection of the power series expansion Equation (54) that all but the first term vanishes, leaving $\mathcal{E}_X(Z) = Z$.

Case: Z in the orthocomplement to $\ker(\text{ad}_X)$. In this space ad_X has a Moore-Penrose generalized inverse. It is most convenient to express $\mathcal{E}_X(Z)$ in vectorized form (c.f. Equation (C11))

$$\text{vec}(\mathcal{E}_X(Z)) = i(U^* \otimes U - I \otimes I)(X^* \otimes I - I \otimes X)^{-1} \times \text{vec}(Z), \quad (62)$$

where the inverse operation is the Moore-Penrose generalized inverse, easily computed by any of the standard computer algebra packages.

General case: We can now compute a general expression for $\mathcal{E}_X(Z)$ by combining these two special cases and our expression for \mathcal{P} , the projector onto $\ker(\text{ad}_X)$. We have

$$\text{vec}(\mathcal{E}_X(Z)) = \text{vec}(\mathcal{E}_X(\mathcal{P}(Z))) + \text{vec}(\mathcal{E}_X(\mathcal{Q}(Z))), \quad (63)$$

where $\mathcal{Q} \equiv \mathcal{I} - \mathcal{P}$ projects onto the orthocomplement of $\ker(\text{ad}_X)$. Using the previous observations we have

$$\begin{aligned} \text{vec}(\mathcal{E}_X(Z)) &= \text{vec}(\mathcal{P})\text{vec}(Z) + \\ &\quad i(U^* \otimes U - I \otimes I)(X^* \otimes I - I \otimes X)^{-1} \times \\ &\quad (I \otimes I - \text{vec}(\mathcal{P}))\text{vec}(Z), \end{aligned} \quad (64)$$

where the inverse is again the Moore-Penrose generalized inverse. Note also that we have

$$\text{vec}(\mathcal{P}) = \sum_j P_j^T \otimes P_j, \quad (65)$$

where the P_j project onto the eigenspaces of X with distinct eigenvalues.

Equations (64) and (65) offer an explicit way of computing the action of \mathcal{E}_X , and thus of making the change of variables from natural Pauli co-ordinates to natural adapted co-ordinates on $T_U SU(2^n)$. In practice, of course, this computation may be rather cumbersome, however it is in principle possible using the approach we have described.

It is easy to invert Equation (64), obtaining

$$\begin{aligned} &\text{vec}(\mathcal{E}_X^{-1}(Z)) \\ &= \text{vec}(\mathcal{P})\text{vec}(Z) \\ &\quad - i(X^* \otimes I - I \otimes X)(U^* \otimes U - I \otimes I)^{-1} \times \\ &\quad (I \otimes I - \text{vec}(\mathcal{P}))\text{vec}(Z), \end{aligned} \quad (66)$$

where the inverse operation is a Moore-Penrose generalized inverse. Using this expression we can explicitly compute the change of variables from natural adapted co-ordinates to natural Pauli co-ordinates on $T_U SU(2^n)$.

IV. THE PAULI GEODESICS

In this section we'll study a class of curves which are geodesics for each of our families of Finsler metrics, $F_{1\Delta}$, $F_{p\Delta}$, F_2 , and F_q . Our study begins in Subsection IV A where we identify some isometries of our Finsler metrics. In Subsection IV B we use these isometries and the geodesic equation to identify a special class of geodesic solutions, which we call *Pauli geodesics*. These solutions are geodesics for *all* the local metrics we have defined, although their lengths may be different for the different local metrics. Examining these Pauli geodesics, we find examples of unitary operators with multiple (indeed, infinitely many) Pauli geodesics passing through them. In Subsection IV C we show that the problem of determining the minimal length Pauli geodesic passing between I and a unitary operation U which is diagonal in the computational basis is equivalent to solving an instance of the closest vector in a lattice problem (CVP). Also in this subsection, we show that if the minimal length curve from I through U is *unique* then it must be a Pauli geodesic, and so the length of the minimal Pauli geodesic will be $d_F(I, U)$. Subsection IV D

uses the connection to CVP to argue that all but a tiny fraction of unitaries diagonal in the computational basis have exponentially long minimal Pauli geodesics. The section concludes in Subsection IV E with a discussion of the results obtained, and some caveats about their implications.

A. Metric isometries

In order to understand the space of solutions to the geodesic equation, it is helpful to first study isometries of the local metric, F , which in turn are reflected in symmetry properties of the geodesics.

What do we mean by an isometry of F ? Suppose $h : M \rightarrow M$ is a diffeomorphism of the Finsler manifold M to itself. If F is a Finsler metric on M , then we say h is an F -isometry if $l_F(s) = l_F(h \circ s)$ for all curves s . It is clear that such an isometry preserves geodesics on the manifold M , i.e. $h \circ s$ is a geodesic if and only if s is a geodesic. It is also straightforward to see that a necessary and sufficient condition for h to be an isometry is that

$$F(s(t), [s]_t) = F((h \circ s)(t), [h \circ s]_t) \quad (67)$$

for all curves s and for all t . Note that $[h \circ s]_t = h_*[s]_t$, where $h_* : T_{s(t)}M \rightarrow T_{h(s(t))}M$ is the linear pushforward map, so this condition may be rewritten:

$$F(x, y) = F(h(x), h_*y) \quad (68)$$

for all $(x, y) \in TM$.

For a local metric $F : T SU(2^n) \rightarrow [0, \infty)$ the condition Equation (68) that h be an isometry is equivalent to the condition

$$F(U, H) = F(h(U), h_*H), \quad (69)$$

where h_* is a superoperator pushing forward the Hamiltonian H representing the tangent at U . When F is right-invariant this may be replaced by the condition

$$F(H) = F(h_*H), \quad (70)$$

where h_* is (implicitly) a function of the location U on $SU(2^n)$, and Equation (70) must be true at all values of U .

It will be convenient to regard h_* as a matrix written with respect to the σ basis. For all our local metrics a sufficient condition for Equation (70) to hold is that h_* be diagonal with respect to this basis, with entries ± 1 . This corresponds to the condition that $F(H)$ does not depend on the sign of the expansion coefficients in $H = \sum_{\sigma} \gamma^{\sigma} \sigma$, but only on their absolute values. We will call any right-invariant local metric with this property a *Pauli-symmetric* local metric. It is clear that $F_{1\Delta}, F_{p\Delta}, F_2$ and F_q are all Pauli-symmetric local metrics. Some of our local metrics admit larger classes of isometries:

- $F_{1\Delta}$: It suffices that h_* be a *signed permutation*, i.e., there is a permutation π of the Pauli matrices such that $h_*(\sigma) = \pm \pi(\sigma)$.
- $F_{p\Delta}$: It suffices that h_* be a block diagonal sum of signed permutations, where the blocks correspond to all those values of σ for which $p(\text{wt}(\sigma))$ takes the same value.
- F_2 : It suffices that h_* be an orthogonal matrix.
- F_q : It suffices that h_* be a block diagonal sum of orthogonal matrices, where the blocks correspond to all those values of σ for which $q(\text{wt}(\sigma))$ takes the same value.

These classes of isometry sometimes impose severe constraints on the form of h . For example, the continuity of h and the fact that $SU(2^n)$ is connected imply that if h_* is a signed permutation for all values of U , then h_* must be a constant. It is not difficult to prove that this constant uniquely determines h_* , so the set of such h_* can be labeled by the signed permutations, of which there are only a finite number. Indeed, it is possible that the class of isometries may be even further constrained: it is not *a priori* clear that given a particular signed permutation there even exists an h such that h_* takes on the value of that signed permutation everywhere.

The problem of obtaining a complete classification of the isometries is an interesting problem in its own right, but it is not our main concern here. Rather, we will construct some explicit examples of isometries h realizing one or more of these conditions, and use those isometries to construct the Pauli geodesics.

Example: adjoint action of the Pauli group. Suppose σ is a generalized Pauli matrix. We can define a corresponding map $h_{\sigma} : SU(2^n) \rightarrow SU(2^n)$ by $h_{\sigma}(U) \equiv \sigma U \sigma^{\dagger}$. A straightforward calculation shows that $h_{\sigma*}(H) = \sigma H \sigma^{\dagger}$, so $h_{\sigma*}$ is indeed diagonal with entries ± 1 , and h_{σ} is an isometry of all our local metrics.

Example: complex conjugation. Define the map $h : SU(2^n) \rightarrow SU(2^n)$ by $h(U) \equiv U^*$. A calculation shows that $h_*(H) = -H^*$, and thus h_* is again diagonal with entries ± 1 . It follows that the map $U \rightarrow U^*$ is an isometry of all our local metrics.

Example: adjoint action of local unitaries. Suppose $W \equiv W_1 \otimes \dots \otimes W_n$ is a local unitary operation on n qubits. Define $h_W : SU(2^n) \rightarrow SU(2^n)$ by $h_W(U) \equiv W U W^{\dagger}$. Then $h_*(H) = W H W^{\dagger}$, whence h_W is an isometry for F_2 and F_q .

Example: adjoint action of the Clifford group. Recall that the n -qubit Clifford group¹² consists of all

¹² Sometimes referred to as the *normalizer* of the Pauli group. See Chapter 10 of [58] for a review of the Clifford group and the associated stabilizer formalism, or [59] for much of the original development of this formalism and its applications in quantum information science.

those n -qubit unitary operations g having the property that $g\sigma g^\dagger$ is a generalized Pauli matrix whenever σ is a generalized Pauli matrix. This group includes many interesting unitary operations, including the controlled-NOT, the Hadamard gate, and the generalized Pauli matrices themselves.

Suppose g is an element of the Clifford group. We can define a corresponding map $h_g : SU(2^n) \rightarrow SU(2^n)$ via $h_g(U) \equiv gUg^\dagger$. We compute the pushforward h_{g*} at U , obtaining $h_{g*}(H) = gHg^\dagger$. Since g is an element of the Clifford group, it follows that h_{g*} is a permutation with respect to the σ co-ordinates, and thus h_g is an isometry of $F_{1\Delta}$ and of F_2 , but not in general of $F_{p\Delta}$ or of F_q .

Example: adjoint action of the unitary group on $SU(2^n)$. Let W be an arbitrary unitary, and define an action $h_W : SU(2^n) \rightarrow SU(2^n)$ by $h_W(U) \equiv WUW^\dagger$. A calculation shows that $h_{W*}(H) = WHW^\dagger$, and thus h_W is an isometry of F_2 , but is not in general an isometry of the other local metrics.

B. Pauli geodesics

The isometries identified in the previous subsection enable us to identify a large class of geodesics which we call *Pauli geodesics*. These geodesics arise as a result of the Pauli group isometry, and thus are geodesics for all the local metrics we have defined, and, indeed, of any Pauli-symmetric local metric.

To construct the Pauli geodesics we begin with a simple proposition.

Proposition 3. *Let M be a Finsler manifold. Suppose $h : M \rightarrow M$ is an isometry and s is a geodesic such that (a) $h(s(0)) = s(0)$, and (b) $h_*([s]_0) = [s]_0$. Then $s = h \circ s$ and $h_*([s]_t) = [s]_t$ for all t .*

Proof: The proof is to observe that s and $h \circ s$ are both geodesics with the same starting point, $h(s(0)) = s(0)$, and the same initial tangent vector $h_*([s]_0) = [s]_0$. The geodesic equation is a second order ordinary differential equation, and thus by the uniqueness of solutions to such equations we deduce that $h \circ s = s$. It follows immediately that $h_*([s]_t) = [s]_t$ for all t . \square

As a simple but useful illustration of the proposition, suppose we have a solution $U(t)$ to the geodesic equation for a Pauli-symmetric Finsler metric, with initial tangent vector corresponding to a Hamiltonian H_0 . Suppose $\sigma H_0 \sigma^\dagger = H_0$ for some generalized Pauli matrix σ . Then Proposition 3 implies that $\sigma U(t) \sigma^\dagger = U(t)$ for all t .

The construction of the Pauli geodesics is based on the stabilizer formalism developed by Gottesman [59]; for a review, see Chapter 10 of [58]. In particular, we suppose $\sigma_1, \dots, \sigma_n$ is a set of stabilizer generators, i.e., independent and commuting generalized Pauli matrices which generate a subgroup S of the full Pauli group. Suppose $H_0 = \sum_{\sigma \in S} h^\sigma \sigma$. Then we claim that the geodesic U with $U(0) = I$ and initial tangent vector corresponding

to H_0 is just $U(t) = \exp(-iH_0t)$, for any Pauli-symmetric Finsler metric. We refer to $U(t)$ as a Pauli geodesic for the Finsler metric.

The first step of the proof is to observe that the Pauli co-ordinates $x^\sigma(t)$ of $U(t)$ are identically zero, unless $\sigma \in S$. To see this, suppose $\sigma \notin S$, and choose $\tilde{\sigma} \in S$ which anticommutes with σ . From our earlier remarks we see that $U(t) = \tilde{\sigma}U(t)\tilde{\sigma}^\dagger$, and thus $x^\sigma(t) = 0$ for all t . We say that a unitary satisfying this condition is *S-invariant*.

We now analyse the geodesic equation, Equation (32), for the co-ordinates x^σ and y^σ with $\sigma \in S$. In particular, because $U(t)$ is guaranteed to be *S*-invariant we may effectively regard F^2 as a function of x^σ and y^σ only for $\sigma \in S$. We have

$$\frac{d}{dt} \left(\frac{\partial F^2}{\partial y^\sigma} \right) = \frac{\partial F^2}{\partial x^\sigma}, \quad (71)$$

where all partial derivatives are evaluated at *S*-invariant unitary matrices. But $\partial F^2 / \partial x^\sigma = 0$ at such an *S*-invariant unitary matrix, since F^2 has no dependence on x^σ , by the commutativity of the elements of S . Substituting this into the right-hand side of Equation (71) and applying the chain rule to the left we obtain:

$$\sum_{\tau \in S} \left(\frac{\partial F^2}{\partial x^\tau \partial y^\sigma} \frac{dx^\tau}{dt} + \frac{\partial F^2}{\partial y^\tau \partial y^\sigma} \frac{dy^\tau}{dt} \right) = 0. \quad (72)$$

But $\frac{\partial F^2}{\partial x^\tau \partial y^\sigma} = 0$, since $\frac{\partial F^2}{\partial x^\tau} = 0$, and thus

$$\sum_{\tau \in S} \frac{\partial F^2}{\partial y^\tau \partial y^\sigma} \frac{dy^\tau}{dt} = 0. \quad (73)$$

Using the invertibility of the Hessian we obtain $\frac{dy^\tau}{dt} = 0$, and thus $x^\tau = c^\tau t$ for some constant c^τ . It follows that the solution to the geodesic equation is

$$U(t) = \exp(-iH_0t), \quad (74)$$

as claimed.

Summing up, for a Pauli-symmetric Finsler metric such as $F_{1\Delta}$, $F_{p\Delta}$, F_2 or F_q , when the initial Hamiltonian H_0 is a sum over terms in a stabilizer subgroup, the corresponding Pauli geodesic solution is just the exponential $U(t) = \exp(-iH_0t)$.

C. Minimal Pauli geodesics and the closest vector in a lattice problem

In this subsection we study the minimal length Pauli geodesics from I to U , where U is diagonal in the computational basis. We show that for any right-invariant Pauli-symmetric Finsler metric this minimal length is equal to the solution of an instance of the closest vector in a lattice problem (CVP). This class of Finsler metrics include all the Finsler metrics of most interest to us: $F_{1\Delta}$, $F_{p\Delta}$, F_2 , and F_q .

Note that the case where U is diagonal in the computational basis corresponds to the case where the stabilizer S contains exactly the products of Pauli I and Z matrices, e.g., for $n = 2$, S contains II, ZI, IZ and ZZ . Exactly analogous results hold for all other choices of stabilizer, but working with this particular stabilizer allows us to make use of certain standard notations and nomenclature, and so avoid the introduction of extra terminology.

One reason for specializing to unitaries diagonal in the computational basis is that it includes a class of unitaries of exceptional interest: those that can be written $U_f = \sum_z (-1)^{f(z)} |z\rangle\langle z|$, where $f(z)$ is a classical Boolean function on the n -bit input z . Kitaev's phase estimation algorithm [60] shows that, given a single ancilla qubit, the computation of U_f requires essentially the same number of quantum gates as computation of the function f on a quantum computer. Thus, bounds on the size of the circuit required to compute U_f are of considerable interest.

Returning to the general case of U diagonal in the computational basis, our goal in this subsection is to study the length of the minimal Pauli geodesic between I and U . Of course, the quantity of real interest to us is the length of the minimal geodesic between I and U , unconstrained by the constraint that it be a Pauli geodesic. Unfortunately, we can't say when it will be true that the minimal length geodesic is going to be a Pauli geodesic. However, the following proposition gives some hopes that this will be the case for some unitaries of interest.

Proposition 4. *Let F be a Pauli-symmetric Finsler metric. Let $U \in SU(2^n)$ be diagonal in the computational basis. Suppose the minimal length geodesic s between I and U is unique, i.e., there is only a single curve s between I and U with $d_F(I, U) = l_F(s)$. Then s must be a Pauli geodesic.*

For the usual model spaces of Riemannian geometry (the sphere, flat Euclidean space, or the hyperbolic space) non-unique minimal paths are quite non-generic, suggesting that the same may be true in the situations of interest to us¹³.

Proof: Let σ be a generalized Pauli matrix containing only Z s and I s. Let s be the minimal length geodesic between I and U . Define $\tilde{s}(t) \equiv \sigma s(t) \sigma^\dagger$. Then \tilde{s} has the same endpoints and length as s , and thus, by the uniqueness of the minimal geodesic, we must have $\tilde{s} = s$. Since this is true for all σ containing only Z s and I s, it follows that $s(t)$ is diagonal in the computational basis for all t , and thus s is a Pauli geodesic. \square

Fixing U , which Pauli geodesics pass from I to U ? To answer this question, choose Hermitian H such that $U = \exp(-iH)$. Let \mathcal{J} be the set of traceless Hermitian matrices which are diagonal in the computational

basis, and have diagonal entries which are integer multiples of 2π . Let $J \in \mathcal{J}$. Then for any such J , the curve $\exp(-i(H - J)t)$ is a Pauli geodesic passing through U .

This freedom to choose J actually exhausts the freedom in the choice of Pauli geodesics¹⁴ passing through U . To see this, suppose $\exp(-iHt)$ and $\exp(-iH't)$ are two Pauli geodesics passing through U at $t = 1$. Then we have $\exp(-iH) = \exp(-iH')$, whence $\exp(i(H' - H)) = I$, since H and H' are both diagonal in the computational basis, and thus commute. However, in order that $\exp(i(H' - H)) = I$, we must have that $J \equiv H - H'$ is traceless (since both H and H' are), and diagonal in the computational basis, with entries which are integer multiples of 2π .

It is straightforward to verify that the set \mathcal{J} has the structure of a lattice, i.e., taking an integer linear combination of elements of \mathcal{J} produces another element of \mathcal{J} . A basis for this lattice is the matrices $2\pi(|z\rangle\langle z| - |0\rangle\langle 0|)$, where $z \neq 0$.

The length of the Pauli geodesic $\exp(-i(H - J)t)$ between I and U is given by $F(H - J)$, so the length of the minimal Pauli geodesic through U is given by:

$$\min_{J \in \mathcal{J}} F(H - J). \quad (75)$$

Thus the problem of finding the minimal length Pauli geodesic is equivalent to finding the lattice vector in \mathcal{J} closest to H according to the $F(\cdot)$ norm on $su(2^n)$. This is the desired connection to the closest vector in a lattice problem.

The connection to lattices also makes it straightforward to construct arbitrarily long geodesics passing through a given unitary. This is true, for example, even in the two-qubit case. Suppose we choose $U = \exp(-i\pi ZZ/2)$, and select $H = \pi ZZ/2 + 2\pi ZI/M$, where M is a positive integer equal to 1 modulo 4. Then $\exp(-iHt)$ is a Pauli geodesic which first passes through U at $t = M$. By making M sufficiently large we can increase the length of this geodesic without bound.

D. Existence of exponentially long minimal Pauli geodesics

In the previous subsection we showed that finding the minimal length Pauli geodesic from I through a diagonal unitary U is equivalent to solving an instance of CVP. In this subsection we'll use this connection to prove that for most such U the minimal length Pauli geodesic is exponential in length. The key is the following proposition, pointed out to the author by Oded Regev:

¹³ Compare, however, the counterexample in Subsection IV E, below.

¹⁴ Note that in analysing the freedom we restrict ourselves to Pauli geodesics $\exp(-iH't)$ for which H' is diagonal in the computational basis. For some very non-generic U it may be that U is diagonal in the computational basis, yet has a Pauli geodesic passing through it for which H' is not diagonal in the computational basis. We shall ignore this possibility.

Proposition 5. Let V be a d -dimensional vector space equipped with the standard Lebesgue measure. Let F be a norm on V , and let $V_F(r)$ be the Lebesgue measure of the unit ball of radius r associated to F . Let \mathcal{J} be a d -dimensional lattice in V , and let M be a matrix whose columns are a lattice basis for \mathcal{J} , so the Lebesgue measure of a unit cell in \mathcal{J} is $\det(M)$. Then if a fraction f ($0 \leq f \leq 1$) of points in V are within a distance r of the lattice we must have

$$f \det(M) \leq V_F(r). \quad (76)$$

Proof: Consider a large volume containing N lattice points. Let R be the region obtained by surrounding each of the N lattice points by the unit ball of radius r according to the norm F . The total Lebesgue measure of the region R is at most $NV_F(r)$. By assumption, in the large N limit R contains at least a fraction f of points in the N unit cells associated to the N lattice points¹⁵, and thus $fN \det(M) \leq NV_F(r)$. Dividing by N gives the desired result. \square

To apply this result, it simplifies matters¹⁶ to vary our earlier approach slightly, moving from $SU(2^n)$ to $U(2^n)$, and defining the local metrics $F_1, F_{1\Delta}, F_p, F_{p\Delta}, F_2, F_q$ analogously to before, but now with a contribution from the $\sigma = I^{\otimes n}$ term. It is not difficult to show that when U is in $SU(2^n)$ it has the same minimal curves regardless of whether we use the formulation of the local metric in $SU(2^n)$ or $U(2^n)$.

In this formulation, Pauli geodesics exist for all our Finsler metrics, and the minimal length Pauli geodesic is found by minimizing $F(H - J)$, where J is in the lattice spanned by matrices of the form $2\pi|z\rangle\langle z|$, which may be rewritten in the more convenient form $2\pi \otimes_{j=1}^n (I + z_j Z_j)/2^n$. Arranged into columns, the corresponding matrix of lattice basis vectors has the form $2\pi H^{\otimes n}/2^{n/2}$, where H is the usual 2×2 Hadamard matrix. Thus the conclusion of Proposition 5 is that

$$f \times \left(\frac{2\pi}{2^{n/2}} \right)^{2^n} \leq V_F(r). \quad (77)$$

Let us analyse what this allows us to conclude about the fraction f of points within a distance r of the lattice, for each of our choices of Finsler metric.

Case: $F_{1\Delta}$. As $\Delta \rightarrow 0$ the unit sphere has volume $V_{F_{1\Delta}}(r) \rightarrow (2r)^{2^n}/(2^n!)$. Applying Stirling's formula, Equation (77) reduces to

$$r \geq \frac{\pi}{e} 2^{n/2} f^{1/2^n} \quad (78)$$

in the $\Delta \rightarrow 0$ limit. In consequence, unless r is exponentially large, at most a doubly exponentially small fraction

of diagonal unitary operators will have minimal Pauli geodesics of length r or less.

Case: $F_{p\Delta}$. Obviously, the minimal length Pauli geodesics for $F_{p\Delta}$ are longer than those for $F_{1\Delta}$, provided the penalty function satisfies $p(j) \geq 1$. Thus, unless r is allowed to be exponentially large, at most a doubly exponentially small fraction of diagonal unitaries will have minimal Pauli geodesics of length r or less.

Case: F_2 . Based on our previous results we expect constant size minimal length Pauli geodesics for F_2 . This expectation is not disappointed. The volume formula in this case is $V_{F_2}(r) = (\sqrt{\pi}r)^{2^n}/(2^n/2)!$. Applying Stirling's formula, and setting $f = 1$, Equation (77) reduces to:

$$\sqrt{\frac{2\pi}{e}} \leq r. \quad (79)$$

Case: F_q . The volume elements is given by

$$V_{F_q} = \frac{(\sqrt{\pi}r)^{2^n}}{(2^n/2)!} \prod_{\sigma} \frac{1}{q(\text{wt}(\sigma))}, \quad (80)$$

where the product is taken over all σ containing only I and Z terms. Applying Stirling's formula, Equation (77) reduces to:

$$f^{1/2^n} \sqrt{\frac{2\pi}{e}} \left(\prod_{\sigma} q(\text{wt}(\sigma)) \right)^{1/2^n} \leq r. \quad (81)$$

We see that provided the penalty function q is chosen appropriately, all but a doubly exponentially small fraction of diagonal unitaries will have minimal Pauli geodesics which are exponentially long. Such a choice is provided, for example, by Equation (28), with k exponentially large.

E. Discussion

In the past few subsections we've explained the construction of the Pauli geodesics, connected the minimal length Pauli geodesic to the solution of an instance of CVP, shown that the minimal length Pauli geodesic is actually the minimal length curve, provided that curve is unique, and proved that most diagonal unitaries have exponential length minimal Pauli geodesics. This subsection injects some words of warning into this otherwise encouraging situation, explaining some significant caveats to our results.

1. On the uniqueness of minimal curves

Based on the standard model spaces of Riemannian geometry (the sphere, Euclidean flat space, or the hyperbolic space), it seems plausible that the minimal geodesics between I and a diagonal unitary U are generally unique, and thus Pauli geodesics. However, this

¹⁵ We neglect finite-size corrections of order sublinear in N .

¹⁶ Analogous results hold for $SU(2^n)$, but the calculations are more complicated, due to the more complex lattice basis.

may not always be the case for F_p , as the following example shows.

Consider the Boolean function $f(z) = f(z_1, \dots, z_n) \equiv z_1 z_2 \dots z_n$, i.e., the AND of the n bits z_1, \dots, z_n , and the associated unitary transformation $U|z\rangle \equiv (-1)^{f(z)}|z\rangle$. Using the connection to CVP, it is easy to verify that for all of our Finsler metrics F the minimal length Pauli geodesic is $\pi F(|1, \dots, 1\rangle\langle 1, \dots, 1|)$.

Consider the case of $F_{p\Delta}$, with the penalty function p chosen as q was in Equation (28). A calculation shows that as $\Delta \rightarrow 0$ the minimal Pauli geodesic has length:

$$\pi \left(k - \frac{2 + n + n^2}{2^{n+1}}(k-1) \right). \quad (82)$$

When k is large, this is dominated by the term πk .

By contrast, the results of Barenco *et al* [28] show that there is a quantum circuit for U containing $O(n^2)$ one- and two-qubit gates. It follows that $d_{F_p}(I, U) \leq cn^2$, for some constant c . To reconcile this result with Equation (82) we see that when k is large, the minimal geodesic between I and U *must not* be a Pauli geodesic, and therefore cannot be unique. This example — which is easily modified to give other examples — suggests that the applicability of Proposition 4 may be limited, at least for some choices of Finsler metric, and highlights the need to develop more tools for the analysis of the distance function $d_F(I, U)$.

2. Classical simulations

We have argued earlier in the paper that it is at least plausible that local metrics such as F_1, F_p and F_q give rise to distance functions $d_F(I, U)$ which are polynomially equivalent to $m_G(U)$. Suppose, for the sake of argument, that we can find a Finsler metric F with this property. Suppose furthermore that for a generic unitary diagonal in the computational basis, the minimal length curve is unique. If this is the case, then for such unitaries there is circuit containing only gates diagonal in the computational basis, and with a size polynomially equivalent to the minimal number of gates required to generate U .

This conclusion would be rather surprising, as such circuits can be simulated with at most a polynomial overhead in the classical circuit model, and it would therefore conflict with the general belief that quantum computers offer a substantial complexity advantage over classical computers.

Of course, there are many potential loopholes in this argument: it makes use of many unstated assumptions (no use of ancillas, no approximation, no uniformity requirement) as well as several steps that, while plausible, could easily turn out to be wrong. I can not at present resolve which of the many possibilities is correct, but it suggests many interesting directions for further research.

V. CONCLUSION

In this paper we have proposed a geometric approach to the problem of proving lower bounds on the number of quantum gates required to synthesize a desired unitary operation. In particular, we have shown that such lower bounds may be provided by the length of the minimal geodesics of certain Finsler metric structures on $SU(2^n)$.

Our main progress in understanding the geodesic structure for these Finsler metrics are the results: (1) a method for computing the geodesic equation explicitly, thus enabling numerical investigations; (2) the construction of a large class of geodesic solutions, which we call Pauli geodesics, passing from the identity I through any unitary U which is diagonal in the computational basis; (3) the demonstration of an equivalence between the problem of finding the minimum length Pauli geodesic between I and U , and the closest vector in a lattice problem (CVP); (4) a proof that when there is a *unique* minimal length geodesic between I and U , then that geodesic must be a Pauli geodesic; and (5) a proof that all but a very small fraction of diagonal unitaries U have minimal length Pauli geodesics which are of exponential length.

To make further progress it will be necessary to obtain more insight into the space of geodesics associated to each of our Finsler metrics. Of course, understanding the space of geodesics associated to a Finsler metric is a difficult problem to solve, even for relatively simple Riemannian spaces, and much of the ongoing work in Riemannian and Finsler geometry is motivated by this problem.

Questions of particular interest include: (a) what are the geodesics; (b) how long are the geodesics, and can we find the minimal length geodesics, or at least a bound on their length; (c) do there exist exponentially long minimal length geodesics, and if so, can we construct some explicit examples, and hence explicit examples of unitary operations requiring an exponential number of gates; and (d) for which (if any) local metric F is the minimal path length $d_F(I, U)$ polynomially equivalent to the size $m_G(U)$ of the minimal quantum circuit synthesizing U ?

Broadening the scope, the results of this paper do not yet address many issues of interest in quantum computational complexity. In particular, our results are constrained entirely to *exact* and *non-uniform* implementations of a unitary operation, while the subject of most interest for quantum computational complexity is approximate and uniform implementations. Also from the point of view of computational complexity, it is desirable to obtain strong results about the impact working qubits (i.e., ancilla) have on minimal path lengths. Finally, it is tempting to speculate on whether a geometric approach along the lines sketched here could ever be powerful enough to resolve complexity class separations. In this vein, it should be noted that results such as the well-known no-go theorem of Razborov and Rudich [61] (see also [62]) suggest that to apply the geometric approach to such separations would require deep insights

into very specific computational problems.

On the flip side, one might ask if these techniques can be of any use in quantum algorithm design, either for recovering existing algorithms, or perhaps in the design of new algorithms. In particular, if we can find a local metric F such that $d_F(I, U)$ is polynomially equivalent to $m_G(U)$, then quantum circuit design may be viewed in terms of the construction of short geodesics between I and the desired unitary operation, i.e., in terms of the solution of a two-point boundary value problem. In a similar vein, application of these ideas to oracle problems and quantum communication complexity may be possible.

Further afield still, one may ask whether a similar approach based on Finsler geometry might be taken in the study of classical computing. *A priori* this idea does not appear particularly promising, as classical computing models are usually formulated in a discrete fashion not amenable to study using the calculus of variations. However, if one reformulates those models using the theory of continuous time, discrete state space Markov chains, I believe it may be possible to apply similar techniques, perhaps along the lines which have been explored in the theory of optimal stochastic control.

APPENDIX A: APPROXIMATING LOCAL METRICS WITH FINSLER METRICS

In this appendix we explain how the local metrics F_1 and F_p , which lack the smoothness and strong convexity properties required by Finsler metrics, can be approximated arbitrarily well by Finsler metrics.

To begin, let's formalize the notion of approximating one local metric by another. Let $F, \tilde{F} : TM \rightarrow [0, \infty)$ be two local metrics on the manifold M . We say F is *metrically equivalent* to \tilde{F} if there exist positive constants A and B such that

$$A F(x, y) \leq \tilde{F}(x, y) \leq B F(x, y) \quad (\text{A1})$$

for all $(x, y) \in TM$. A little thought shows that this definition, which appears asymmetric in F and \tilde{F} , is actually symmetric. It is also easy to see that if F and \tilde{F} are metrically equivalent then they satisfy

$$A d_F(x_1, x_2) \leq d_{\tilde{F}}(x_1, x_2) \leq B d_F(x_1, x_2), \quad (\text{A2})$$

for all x_1 and $x_2 \in M$.

Our goal in this appendix is to construct Finsler metrics $F_{1\Delta}$ and $F_{p\Delta}$ which are metrically equivalent to F_1 and F_p , respectively, for sufficiently small values of the positive parameter Δ . Furthermore, as $\Delta \rightarrow 0$ it turns out that $A \rightarrow 1$ and $B \rightarrow 1$ for both classes of metrics, so Equation (A2) tells us that the notion of length given by $F_{1\Delta}$ and $F_{p\Delta}$ approaches that given by F_1 and F_p .

Our strategy in constructing the approximating Finsler metrics is to first study the problem of finding Minkowski

norms N_Δ which approximate a given norm¹⁷ N on \mathbb{R}^d . Once we understand this problem it is straightforward to construct the appropriate Finsler metrics.

Constructing Minkowski norms with suitable properties does not seem easy to do directly, in large part because of the positive homogeneity condition for norms. We will take a more indirect approach to the definition, defining norms in terms of their indicatrices, i.e., their unit spheres. This material, described in Subsection A 1, is well-known in the Finsler geometry literature (see, e.g. [45]), and our discussion merely outlines the major facts. The exception is Proposition 7, which seems to be a well-known folklore result, but which I have not found explicitly in the prior literature. Consequently, a proof is included. Subsection A 2 uses this background to construct the desired classes of approximating Finsler metrics.

1. The indicatrix and the implicit definition of Minkowski norms

The following proposition gives a convenient way of defining smooth norms in terms of a function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ which is *not* necessarily positively homogeneous. To state the proposition we define S_g to be the set of points y such that $g(y) = 1$. We will use g to construct a norm N_g whose indicatrix is S_g .

Proposition 6. *Suppose $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is smooth, convex, satisfies $g(0) < 1$, and is such that S_g is compact. Then the function N_g defined by the equations*

$$N_g(0) = 0; \quad (\text{A3})$$

$$g\left(\frac{y}{N_g(y)}\right) = 1, \text{ provided } y \neq 0. \quad (\text{A4})$$

exists, is uniquely defined, is smooth away from the origin, and is a norm with indicatrix S_g .

Proof: This is easily proved, and a well-known result of Finsler geometry. See, for example, [45] for an outline of the proof. The only non-trivial step is an application of the implicit function theorem (see, e.g., Chapter 7 of [43]) to the implicit definition (A4) of N_g , in order to obtain the smoothness condition for N_g . \square

When does N_g obey the strong convexity constraint? The following proposition gives a simple criterion for N_g to be strongly convex.

Proposition 7. *Suppose $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is such that the matrix G with entries $\left(\frac{\partial g}{\partial y^j \partial y^k}\right)$ is strictly positive for any $y \neq 0$. Then the norm N_g defined by Equations (A3) and (A4) is strongly convex.*

¹⁷ Note that in keeping with standard usage in Finsler geometry we only require norms to be positively homogeneous, not homogeneous, as is usually stipulated in other contexts.

Proof: To simplify notation we write $N = N_g$. We begin by differentiating the implicit definition Equation (A4) with respect to y^j , obtaining

$$N_{,j}(y) = \frac{N(y)g_{,j}(\hat{y})}{(\nabla_{\hat{y}}g \cdot y)}, \quad (\text{A5})$$

where $_{,j}$ denotes partial differentiation with respect to y^j , $\hat{y} \equiv y/N(y)$, and $\nabla_{\hat{y}}$ denotes the usual gradient operator, evaluated at \hat{y} . Differentiating again, we obtain:

$$\begin{aligned} N_{,jk}(y) &= \frac{g_{,jk}(\hat{y})}{\nabla_{\hat{y}}g \cdot y} + \frac{g_{,j}(\hat{y})g_{,k}(\hat{y})\sum_{lm}g_{,lm}(\hat{y})y^ly^m}{(\nabla_{\hat{y}}g \cdot y)^3} \\ &\quad - \frac{\sum_l(g_{,j}(\hat{y})g_{,kl}(\hat{y}) + g_{,k}(\hat{y})g_{,jl}(\hat{y}))y^l}{(\nabla_{\hat{y}}g \cdot y)^2}. \end{aligned} \quad (\text{A6})$$

We also obtain

$$N_{,jk}^2(y) = 2N(y)N_{,jk}(y) + 2N_{,j}(y)N_{,k}(y). \quad (\text{A7})$$

Combining these results we obtain the Hessian:

$$\begin{aligned} H_{jk}(y) &= \frac{N_{,jk}}{\nabla g \cdot y} + \frac{N_{,j}g_{,k}}{(\nabla g \cdot y)^3} \left(\sum_{lm}g_{,lm}y^ly^m + N\nabla g \cdot y \right) \\ &\quad - \frac{N\sum_l(g_{,j}g_{,kl} + g_{,k}g_{,jl})y^l}{(\nabla g \cdot y)^2}, \end{aligned} \quad (\text{A8})$$

where, to simplify notation, it is implicit that all derivatives of g are evaluated at \hat{y} , and N is evaluated at y .

Examining Equation (A8), we see that the contribution from the first term on the right-hand side is strictly positive, since both N and $\nabla g \cdot y$ are strictly positive, and $g_{,jk}$ is strictly positive, by assumption. The contribution from the second term is positive, since it is a positive scalar multiple of the positive matrix with components $g_{,j}g_{,k}$. Thus the sum of the first two terms is strictly positive. The final term of Equation (A8) is more problematic, due to the presence of the minus sign.

The resolution is to make a linear change of variables which simplifies the Hessian. In particular, we make a linear change of variables so that $y = (\alpha, 0, 0, \dots, 0)$, and $\nabla g = (\beta, 0, 0, \dots, 0)$. It is not difficult to see that such a linear change of variables is always possible, and moreover does not affect whether or not the Hessian is strictly positive. It does, however, make the analysis simpler. In particular, observe that by homogeneity we have:

$$N^2(\alpha, 0, \dots, 0) = \alpha^2N(1, 0, \dots, 0) \quad (\text{A9})$$

$$N_{,1}^2(\alpha, 0, \dots, 0) = 2\alpha N(1, 0, \dots, 0) \quad (\text{A10})$$

$$N_{,11}^2(\alpha, 0, \dots, 0) = 2N(1, 0, \dots, 0). \quad (\text{A11})$$

Observe also that for $j = 2, \dots, d$ we have $N_{,j}^2(\alpha, 0, \dots, 0) = 0$, since $\nabla_y g = (\beta, 0, \dots, 0)$. The homogeneity of N then implies that $N_{,j}^2(\alpha, 0, \dots, 0) = 0$ for all α , and thus

$$N_{,1j}^2(\alpha, 0, \dots, 0) = N_{,j1}^2(\alpha, 0, \dots, 0) = 0. \quad (\text{A12})$$

In consequence, the Hessian matrix has the form:

$$\begin{bmatrix} N(1, 0, \dots, 0) & 0 \\ 0 & H_{jk} \end{bmatrix}, \quad (\text{A13})$$

where the H_{jk} are for $j, k = 2, \dots, d$. But for such values of j and k we have $g_{,j} = g_{,k} = 0$ and thus by Equation (A8) we have $H_{jk} = N_{,jk}/\nabla g \cdot y$, whence the Hessian matrix has the form:

$$\begin{bmatrix} N(1, 0, \dots, 0) & 0 \\ 0 & N_{,jk}/\nabla g \cdot y \end{bmatrix}. \quad (\text{A14})$$

The strict positivity of this matrix now follows from our assumption that the matrix whose entries are the $g_{,jk}$ is strictly positive, and the fact that any submatrix of a strictly positive matrix is strictly positive. \square

We can sum up the results of the last two propositions in a single theorem.

Theorem 4. Suppose $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is smooth, convex, satisfies $g(0) < 1$, is such that S_g is compact, and the matrix G with entries $\left(\frac{\partial g}{\partial y^j \partial y^k}\right)$ is strictly positive for any $y \neq 0$. Then the function N_g defined by the equations

$$N_g(0) = 0; \quad (\text{A15})$$

$$g\left(\frac{y}{N_g(y)}\right) = 1, \text{ provided } y \neq 0 \quad (\text{A16})$$

exists, is uniquely defined, and is a Minkowski norm with indicatrix S_g .

2. Constructing the approximating Finsler metrics

We now have all the tools in place to construct the desired Finsler metrics. In particular, we now explicitly construct $F_{p\Delta}$. The family of Finsler metrics $F_{1\Delta}$ follow as the special case where $p(j) = 1$ for all j .

Consider first the function of a single variable $g(y) \equiv \sqrt{\Delta^2 + y^2}$. This is a smooth and strictly convex function, but as $\Delta \rightarrow 0$ it approaches $|y|$. This suggests defining (y is now a $(4^n - 1)$ -dimensional vector):

$$g_{p\Delta}(y) \equiv \sum_{\sigma} p(\text{wt}(\sigma))\sqrt{\Delta^2 + (y^{\sigma})^2}. \quad (\text{A17})$$

Provided Δ is sufficiently small, it is easy to verify that $g_{p\Delta}$ is smooth, convex, satisfies $g(0) < 1$, and is such that S_g is compact. A calculation shows that

$$\frac{\partial g_{p\Delta}}{\partial y^{\sigma} \partial y^{\tau}} = \frac{p(\text{wt}(\sigma))\Delta^2 \delta_{\sigma\tau}}{(\Delta^2 + (y^{\sigma})^2)^{3/2}}, \quad (\text{A18})$$

which clearly specifies a strictly positive matrix. Thus $g_{p\Delta}$ induces a Minkowski norm $N_{p\Delta} \equiv N_{g_{p\Delta}}$.

It is intuitively clear that $N_{p\Delta}$ tends to the norm $N_p(y) \equiv \sum_{\sigma} p(\text{wt}(\sigma))|y^{\sigma}|$ as Δ goes to zero. We can

make this intuition quantitative as follows. Define $P \equiv \sum_{\sigma} p(\text{wt}(\sigma))$ and observe that

$$N_p(y) \leq g_{p\Delta}(y) \leq N_p(y) + P\Delta, \quad (\text{A19})$$

where the first inequality follows from the fact that $|y| \leq \sqrt{\Delta^2 + y^2}$, and the second inequality follows from the fact that $\sqrt{\Delta^2 + y^2} \leq |y| + \Delta$. These inequalities imply:

$$\begin{aligned} N_p\left(\frac{y}{N_{p\Delta}(y)}\right) &\leq g_{p\Delta}\left(\frac{y}{N_{p\Delta}(y)}\right) \leq N_p\left(\frac{y}{N_{p\Delta}(y)}\right) \\ &\quad + P\Delta. \end{aligned} \quad (\text{A20})$$

Observing that $g_{p\Delta}(y/N_{p\Delta}(y)) = 1$, multiplying by $N_{p\Delta}(y)$, and rearranging gives

$$N_p(y) \leq N_{p\Delta}(y) \leq \frac{N_p(y)}{1 - P\Delta}. \quad (\text{A21})$$

Thus provided $\Delta \ll 1/P$ we see that $N_p(y) \approx N_{p\Delta}(y)$.

Summing up, we have defined $g_{p\Delta} : \mathbb{R}^{4^n-1} \rightarrow \mathbb{R}$ by $g_{p\Delta}(y) \equiv \sum_{\sigma} p(\text{wt}(\sigma))\sqrt{\Delta^2 + (y^{\sigma})^2}$. Provided $\Delta < 1/P$, where $P \equiv \sum_{\sigma} p(\text{wt}(\sigma))$, there exists a unique function $N_{p\Delta} : \mathbb{R}^{4^n-1} \rightarrow \mathbb{R}$ defined by $N_{p\Delta}(0) \equiv 0$ and for all other y by

$$g_{p\Delta}\left(\frac{y}{N_{p\Delta}(y)}\right) = 1. \quad (\text{A22})$$

This function $N_{p\Delta}$ is a Minkowski norm which approximates N_p well in the sense that

$$N_p(y) \leq N_{p\Delta}(y) \leq \frac{N_p(y)}{1 - P\Delta}. \quad (\text{A23})$$

We use $N_{p\Delta}$ to define a Finsler metric $F_{p\Delta}$ on $SU(2^n)$, via

$$F_{p\Delta}(U, y) \equiv N_{p\Delta}(\gamma), \quad (\text{A24})$$

where γ is the $(4^n - 1)$ -dimensional vector whose components are the natural U -adapted co-ordinates for $y \in T_U SU(2^n)$. By construction this is a family of Minkowski norms on $SU(2^n)$. To see that $F_{p\Delta}$ is Finsler, we need only prove that it is a smooth function of U . This is intuitively clear. A rigorous proof follows from the results of Section III, which show how to explicitly calculate $F_{p\Delta}$. Note that $F_{p\Delta}$ approximates F_p well in the sense that:

$$F_p(U, y) \leq F_{p\Delta}(U, y) \leq \frac{F_p(U, y)}{1 - P\Delta}. \quad (\text{A25})$$

Using results of Ghomi [63] on smoothing of convex polytopes it is possible to extend the approximation described here to show that any right-invariant local metric can be approximated arbitrarily well by a right-invariant Finsler metric. Ghomi's results even imply that any symmetries in the local metric can be retained by the approximating Finsler metric. I expect that it is possible to extend Ghomi's results to approximation of arbitrary

local metrics by Finsler metrics, but have not verified this assertion. The main disadvantage of Ghomi's constructions — a very substantial disadvantage from our point of view, and the reason they are not used in this paper — is that they involve substantially more complex computations than in the approach we have used to approximate F_1 and F_p .

APPENDIX B: PROOF OF THEOREM 2

To prove Theorem 2 we make use of the following lemma:

Lemma 1. *The equation $\vec{X} + \vec{X} \times \vec{A} = \vec{B}$, where \vec{A}, \vec{B} and \vec{X} are all three-dimensional real vectors, has the unique solution*

$$\vec{X} = \frac{1}{1 + \|\vec{A}\|^2} \left(\vec{B} + \vec{A} \vec{A} \cdot \vec{B} + \vec{A} \times \vec{B} \right). \quad (\text{B1})$$

Proof of Lemma 1: This solution is easily verified by hand or using any of the standard computer algebra packages. \square

Proof of Theorem 2: Fixing \vec{y} it is clear that some \tilde{y} satisfying Equation (44) must exist. All that we have to do is verify that \tilde{y} has the form specified in Equation (46). To do this we simply compare the order t terms on the left- and right-hand sides of Equation (44). Beginning with the right-hand side we see that the term of order t is:

$$\begin{aligned} &-it(\tilde{y} \cdot \sigma) \exp(-i\vec{x} \cdot \sigma) = \\ &-t[\sin(\|\vec{x}\|)\hat{x} \cdot \tilde{y}I + i(\cos(\|\vec{x}\|)\tilde{y} + \sin(\|\vec{x}\|)\tilde{y} \times \hat{x}) \cdot \sigma]. \end{aligned} \quad (\text{B2})$$

To compute the terms of order t obtained from the left-hand side of Equation (44) it helps to define $\vec{z} \equiv \vec{x} + t\vec{y}$. Simple calculations show that the following relationships hold, all to first order in t :

$$\|\vec{z}\| = \|\vec{x}\| + t\hat{x} \cdot \vec{y} \quad (\text{B3})$$

$$\cos(\|\vec{z}\|) = \cos(\|\vec{x}\|) - t \sin(\|\vec{x}\|)\hat{x} \cdot \vec{y} \quad (\text{B4})$$

$$\sin(\|\vec{z}\|) = \sin(\|\vec{x}\|) + t \cos(\|\vec{x}\|)\hat{x} \cdot \vec{y} \quad (\text{B5})$$

$$\hat{z} = \hat{x} + \frac{t}{\|\vec{x}\|}\vec{y}_{\perp}, \quad (\text{B6})$$

where $\vec{y}_{\perp} \equiv \vec{y} - \hat{x} \cdot \vec{y}\hat{x}$ is the component of \vec{y} orthogonal to \vec{x} . Expanding the left-hand-side of Equation (44) out gives

$$\begin{aligned} &\cos(\|\vec{z}\|)I - i \sin(\|\vec{z}\|)\hat{z} \cdot \sigma \\ &= (\cos(\|\vec{x}\|) - t \sin(\|\vec{x}\|)\hat{x} \cdot \vec{y})I \end{aligned} \quad (\text{B7})$$

$$\begin{aligned} &-i(\sin(\|\vec{x}\|) + t \cos(\|\vec{x}\|)\hat{x} \cdot \vec{y}) \left(\hat{x} + \frac{t}{\|\vec{x}\|}\vec{y}_{\perp} \right) \cdot \sigma. \end{aligned} \quad (\text{B8})$$

It follows that the term of order t on the left-hand side of Equation (44) is

$$-t[\sin(\|\vec{x}\|)\hat{x} \cdot \vec{y} I + i(\cos(\|\vec{x}\|)\hat{x} \cdot \vec{y} \hat{x} + \text{sinc}(\|\vec{x}\|)\vec{y}_\perp) \cdot \sigma]. \quad (\text{B9})$$

Comparing the terms in Equations (B2) and (B9) we obtain two equations:

$$\vec{x} \cdot \vec{y} = \vec{x} \cdot \tilde{y} \quad (\text{B10})$$

$$\begin{aligned} & \cos(\|\vec{x}\|)\hat{x} \cdot \vec{y} \hat{x} + \text{sinc}(\|\vec{x}\|)\vec{y}_\perp \\ &= \cos(\|\vec{x}\|)\tilde{y} + \sin(\|\vec{x}\|)\tilde{y} \times \hat{x}. \end{aligned} \quad (\text{B11})$$

We will use these equations to solve for \vec{y} in terms of \tilde{y} , and vice versa. Let us first express \vec{y} in terms of \tilde{y} . To do this it helps to note that $\vec{y}_\perp = \vec{y} - \hat{x} \cdot \vec{y} \hat{x} = \vec{y} - \hat{x} \cdot \tilde{y} \hat{x}$, by Equation (B10). Substituting this expression for \vec{y}_\perp into Equation (B11), multiplying by $1/\text{sinc}(\|\vec{x}\|)$ and simplifying we obtain

$$\vec{y} = \tilde{y}_\parallel + \|\vec{x}\| \cot(\|\vec{x}\|) \tilde{y}_\perp + \tilde{y} \times \vec{x}, \quad (\text{B12})$$

where $\tilde{y}_\parallel \equiv \hat{x} \cdot \tilde{y} \hat{x}$ is the component of \tilde{y} parallel to \hat{x} , and $\tilde{y}_\perp \equiv \tilde{y} - \tilde{y}_\parallel$ is the component of \tilde{y} orthogonal to \hat{x} . This is the desired expression for \vec{y} in terms of \vec{x} and \tilde{y} .

To obtain \tilde{y} in terms of \vec{y} and \vec{x} , we again start from Equation (B10) and (B11). Multiplying Equation (B11) by $1/\cos(\|\vec{x}\|)$ we see it is equivalent to

$$\tilde{y} + \tan(\|\vec{x}\|)\tilde{y} \times \hat{x} = \hat{x} \cdot \vec{y} \hat{x} + \frac{\tan(\|\vec{x}\|)}{\|\vec{x}\|} \tilde{y}_\perp. \quad (\text{B13})$$

Applying Lemma 1 and simplifying the resulting expression we obtain

$$\tilde{y} = \vec{y}_\parallel + \text{sinc}(2\|\vec{x}\|)\vec{y}_\perp + \text{sinc}^2(\|\vec{x}\|)\vec{x} \times \vec{y}_\perp, \quad (\text{B14})$$

where $\vec{y}_\parallel \equiv \hat{x} \cdot \vec{y} \hat{x}$ is the component of \vec{y} in the \hat{x} direction. This is the desired expression for \tilde{y} in terms of \vec{x} and \vec{y} . \square

APPENDIX C: VECTORIZING MATRIX EQUATIONS

In this appendix we give a brief introduction to the *vectorizing* technique, which can be used to convert matrix equations into equivalent vector equations. The treatment is based on [64], which is, in turn, based on material in Chapter 4 of Horn and Johnson [65].

The vectorizing technique is based on a mathematical operation known as the *vec* operation, which may be applied to either a matrix or a superoperator. When *vec* is applied to a matrix, it produces as output the vector formed by stacking all the columns of the matrix up on top of one another. More formally, let $M_{m,n}$ denote the space of $m \times n$ complex matrices. Let $A \in M_{m,n}$. Then we define *vec*(A) to be the mn -dimensional vector

formed by stacking all the columns of A up on top of one another. For example, we have:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \Rightarrow \text{vec}(A) = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}. \quad (\text{C1})$$

We call *vec*(A) the *vectorized* form of the matrix A .

The operation *vec* has many useful properties, and we note only a few here (see [64, 65] for more). In particular, if $A, B \in M_{m,n}$ then *vec*(A) = *vec*(B) if and only if $A = B$. Furthermore, for every mn -dimensional vector v there exists a unique matrix $M \in M_{m,n}$ such that *vec*(M) = v . We will write $M = \text{unvec}(v)$, and speak of *unvectorizing* v to obtain M . Note that for this operation to be well-defined we need to specify m and n .

Why define *vec*? The answer is that it provides an algebraically and computationally convenient way of making explicit the structure of $M_{m,n}$ as a vector space.

The key algebraic fact about *vec* can be understood physically as a connection with maximally entangled states. Let $A \in M_{m,n}$, and let quantum systems Q_1 and Q_2 both have dimension n . Define an (unnormalized) maximally entangled state of $Q_1 Q_2$ by

$$|ME_n\rangle \equiv \sum_j |j\rangle |j\rangle \quad (\text{C2})$$

where the $|j\rangle$ are fixed orthonormal bases for systems Q_1 and Q_2 , respectively. (We won't bother to distinguish the two bases notationally, although they are, of course, distinct bases.) Regarding the matrix A as being defined in the basis $|j\rangle$ for Q_2 , we have the identity

$$\text{vec}(A) = (I_n \otimes A)|ME_n\rangle, \quad (\text{C3})$$

where I_n is the $n \times n$ identity matrix. We will omit the subscript n when its value is clear from context. To prove Equation (C3) note that by linearity it suffices to prove the identity when $A = |j\rangle \langle k|$. The proof is completed by verifying that $\text{vec}(|j\rangle \langle k|) = |k\rangle |j\rangle$ and $(I \otimes |j\rangle \langle k|)|ME_n\rangle = |k\rangle |j\rangle$.

The identity Equation (C3) has an extremely useful generalization, which Horn and Johnson ascribe to Roth [66]. The proof is straightforward algebraic manipulation, and thus is omitted.

Lemma 2 (Roth's lemma). *When $A \in M_{l,m}$, $B \in M_{m,n}$, $C \in M_{n,p}$, we have*

$$\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B). \quad (\text{C4})$$

Roth's lemma is extremely helpful in the analysis of linear matrix equations, such as $\sum_j A_j X B_j = C$. From Roth's lemma, we see that this is equivalent to the equation

$$\sum_j (B_j^T \otimes A_j)\text{vec}(X) = \text{vec}(C), \quad (\text{C5})$$

which may be solved using standard techniques.

This discussion suggests defining a vectorized form for a superoperator. In particular, given a superoperator $\mathcal{L}(\cdot)$, we define a vectorized form of \mathcal{L} as follows. First, note that \mathcal{L} can always be written in the form $\mathcal{L}(X) = \sum_j A_j X B_j$, for some set of matrices A_j and B_j . Then the vectorized form of \mathcal{L} is defined by

$$\text{vec}(\mathcal{L}) \equiv \sum_j B_j^T \otimes A_j. \quad (\text{C6})$$

It is not difficult to show that $\text{vec}(\mathcal{L})$ defined in this way is unique, i.e., it does not depend on the particular representation in terms of a set of A_j and B_j operators. By Roth's lemma we have

$$\text{vec}(\mathcal{L})\text{vec}(X) = \text{vec}(\mathcal{L}(X)). \quad (\text{C7})$$

With these definitions we see that the vectorized forms of the superoperators \mathcal{I} and ad_X are given by

$$\text{vec}(\mathcal{I}) = I \otimes I \quad (\text{C8})$$

$$\text{vec}(\text{ad}_X) = I \otimes X - X^* \otimes I, \quad (\text{C9})$$

where in the second line we assumed that X is Hermitian, and thus $X^T = X^*$.

The vec operation for superoperators has all the algebraic properties one would expect. It is linear in \mathcal{L} , and

a homomorphism, i.e., $\text{vec}(\mathcal{L}_1 \circ \mathcal{L}_2) = \text{vec}(\mathcal{L}_1)\text{vec}(\mathcal{L}_2)$. That is, vec converts composition of linear superoperators into matrix multiplication. As a consequence, we see that if $f(x) = \sum_{j=0}^{\infty} f_j x^j$, then $\text{vec}(f(\mathcal{L})) = f(\text{vec}(\mathcal{L}))$. Using this result, followed by Equation (C9), we deduce that

$$\text{vec}(\exp(-i\text{ad}_X)) = U^* \otimes U, \quad (\text{C10})$$

where $U = \exp(-iX)$. It follows that the operation \mathcal{E}_X defined in Subsection III E has vectorized form:

$$\text{vec}(\mathcal{E}_X) = \frac{U^* \otimes U - I \otimes I}{-i(I \otimes X - X^* \otimes I)}. \quad (\text{C11})$$

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